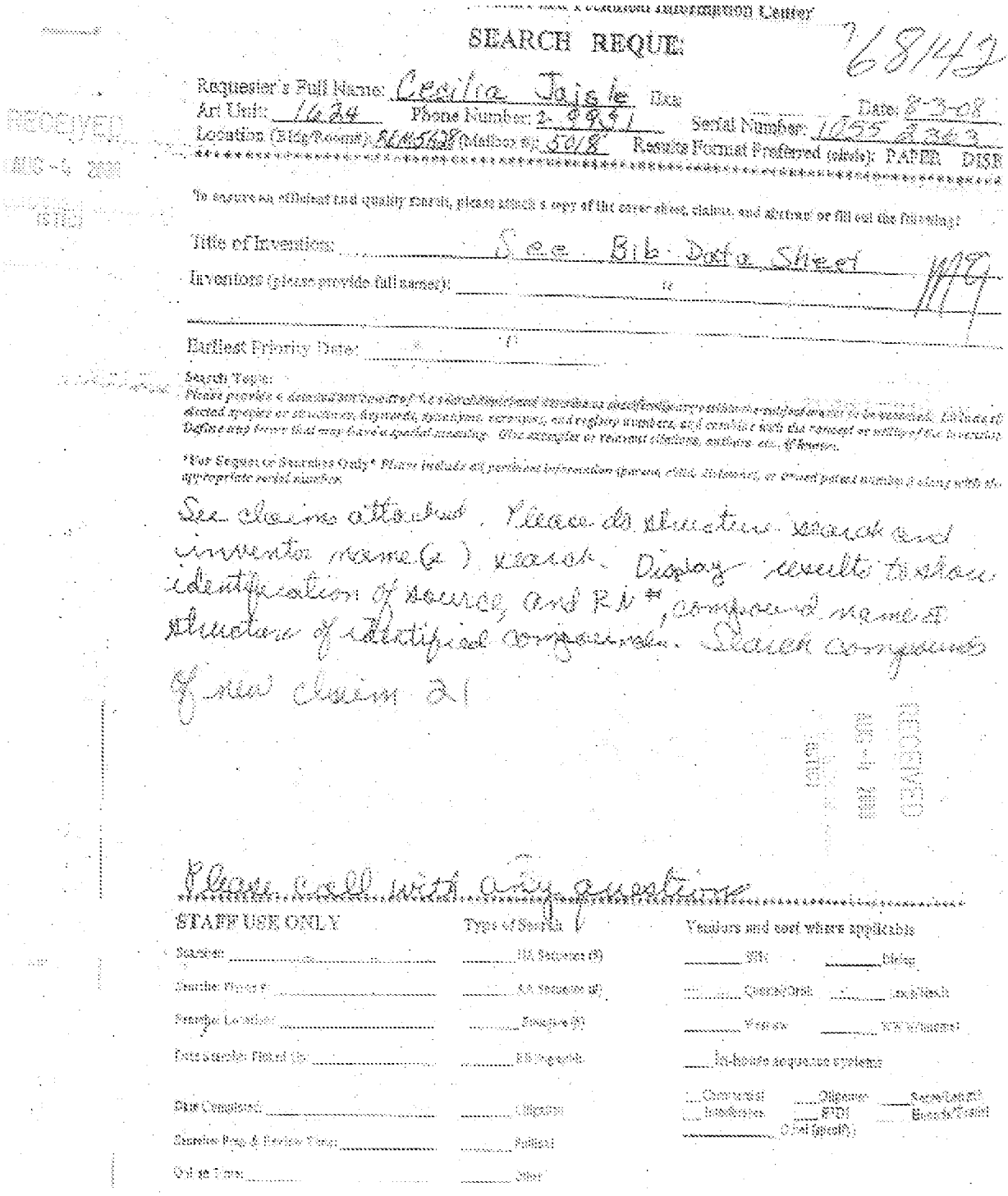

SEARCH REQUE

Requester's Full Name: Cecilia Tajo Date: 8-3-08
Art Unit: 1624 Phone Number: 2-0951 Serial Number: 10/552363
Location (Bldg/Room): RNB 5B48 Mail Box #: 5B48 Results Format Preferred (circle): PAPER DISK

To assure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

Title of Invention: See Bib. Data Sheet

Inventors (please provide full names):

Earliest Priority Date:

Search Topic:
Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known.

For Sequence or Structure Only Please include all pertinent information (parent case, text search, or known publication number) along with the appropriate serial number.

See claims attached. Please do structure search and inventor name(s) search. Display result to show identification of source and RN#, compound name & structure of identified compounds. Search compounds of new claim 21

Please call with any questions

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Type of Search

Vendors and cost where applicable

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DICTIONARY FILE UPDATES: 2 AUG 2008 HIGHEST RN 1037774-47-2

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TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

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http://www.cas.org/support/stngen/stndoc/properties.html

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FILE COVERS 1907 - 4 Aug 2008 VOL 149 ISS 6
FILE LAST UPDATED: 3 Aug 2008 (20080803/ED)

ZCAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

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This file contains CAS Registry Numbers for easy and accurate substance identification.
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reclassified documents, but they can be identified by
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20071130/UPIC and 20080401/UPIC.
ECLA reclassifications to April and US national classifications to
the end of January 2008 have also been loaded. Update dates
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PROCESSING COMPLETED FOR L78
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L79  ANSWER 1 OF 43  ZCAPLUS  COPYRIGHT 2008 ACS on STN DUPLICATE 1
ACCESSION NUMBER:         2008:703598  ZCAPLUS  Full-text
TITLE:                    Inhibition of Invariant Chain Processing,
                          Antigen-Induced Proliferative Responses, and the
                          Development of Collagen-Induced Arthritis and
                          Experimental Autoimmune Encephalomyelitis by a Small
                          Molecule Cysteine Protease Inhibitor
AUTHOR(S):                Podolin, Patricia L.; Bolognese, Brian J.; Carpenter,
                          Donald C.; Davis, T. Gregg; Johanson, Roy A.; Fox,
                          Josephine H.; Long, Edward, III; Dong, Xiaoyang;
                          Marquis, Robert W.; LoCastro, Stephen M.; Terfloth,
                          Gerald J.; Kurali, Edit; Peterson, John J.; Smith,
                          Brian R.; McQueney, Michael S.; Yamashita, Dennis
                          S.; Capper-Spudich, Elizabeth A.
CORPORATE SOURCE:         Respiratory and Inflammation Center of Excellence for
                          Drug Discovery, GlaxoSmithKline, King of Prussia, PA,
                          19406, USA
SOURCE:                   Journal of Immunology (2008), 180(12), 7989-8003
                          CODEN: JOIMA3; ISSN: 0022-1767
PUBLISHER:                American Association of Immunologists
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
AB    Members of the papain family of cysteine proteases (cathepsins) mediate late
      stage processing of MHC class II-bound invariant chain (Ii), enabling
      dissociation of Ii, and binding of antigenic peptide to class II mols.
      Recognition of cell surface class II/Ag complexes by CD4+ T cells then leads
      to T cell activation.  Herein, we demonstrate that a pan-active cathepsin
      inhibitor, SB-331750, attenuated the processing of whole cell Ii p10 to CLIP
      by Raji cells, and DBA/1, SJL/J, and C57BL/6 splenocytes.  In Raji cells and
      C57BL/6 splenocytes, SB-331750 inhibited class II-associated Ii processing and
      reduced surface class II/CLIP expression, whereas in SB-331750-treated DBA/1
      and SJL/J splenocytes, class II-associated Ii processing intermediates were
      undetectable.  Incubation of lymph node cells/splenocytes from collagen-primed
      DBA/1 mice and myelin basic protein-primed SJL/J mice with Ag in the presence
      of SB-331750 resulted in concentration-dependent inhibition of Ag-induced
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proliferation. In vivo administration of SB-331750 to DBA/1, SJL/J, and C57BL/6 mice inhibited splenocyte processing of whole cell Ii p10 to CLIP. Prophylactic administration of SB-331750 to collagen-immunized/boosted DBA/1 mice delayed the onset and reduced the severity of collagen-induced arthritis (CIA), and reduced paw tissue levels of IL-1β and TNF-α. Similarly, treatment of myelin basic protein-primed SJL/J lymph node cells with SB-331750 delayed the onset and reduced the severity of adoptively transferred exptl. autoimmune encephalomyelitis (EAE). Therapeutic administration of SB-331750 reduced the severity of mild/moderate CIA and EAE. These results indicate that pharmacol. inhibition of cathepsins attenuates CIA and EAE, potentially via inhibition of Ii processing, and subsequent Ag-induced T cell activation.

CC 1-7 (Pharmacology)

REFERENCE COUNT: 65 THERE ARE 65 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 2 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 2

ACCESSION NUMBER: 2007:591360 ZCAPLUS Full-text

DOCUMENT NUMBER: 147:31135

TITLE: Pyrimidinone derivatives as calcilytic compounds and their preparation, pharmaceutical compositions and use as calcium receptor inhibitors for treatment of bone and mineral diseases

INVENTOR(S): Ku, Thomas Wen Fu; Lin, Hong; Luengo, Juan I.; Marquis, Robert W., Jr.; Ramanjulu, Joshi M.; Trout, Robert; Yamashita, Dennis S.

PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA

SOURCE: PCT Int. Appl., 251pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2007062370	A2	20070531	WO 2006-US61150		20061121
WO 2007062370	A3	20071122			
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AU 2006318275	A1	20070531	AU 2006-318275		20061121
PRIORITY APPLN. INFO.:			US 2005-738731P	P	20051122
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			WO 2006-US61150	W	20061121

OTHER SOURCE(S): MARPAT 147:31135

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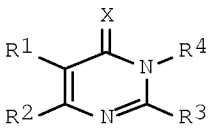

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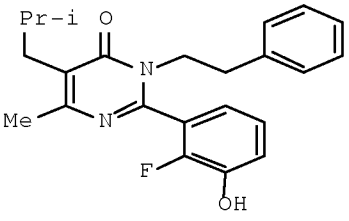


II

AB Novel calcilytic compds. of formula I, pharmaceutical compns., methods of synthesis and methods of using them are provided. Compds. of formula I wherein C is O and S; R1 and R2 are independently H, halo, CN, C1-10 alkyl, C2-6 alkenyl, cycloalkyl, (hetero)aryl, etc.; R3 is (un)substituted (hetero)aryl; R4 is (un)substituted (hetero)aryl, (un)substituted heterocyclyl, (un)substituted cycloalkyl-C1-4 alkyl, etc.; and their pharmaceutically acceptable salts thereof, are claimed. Example compound II was prepared by alkylation of Et 3-oxobutanoate with 3-bromo-2-methyl-1-propene; the resulting Et 2-acetyl-4-methyl-4-pentenoate underwent amidation with phenethylamine to give 2-acetyl-4-methyl-N-(phenethyl)-4- pentenamide, which underwent hydrogenation to give 2-acetyl-4-methyl-N- (phenethyl)-4-pentanamide, which underwent cyclization with 2-fluoro-3-methoxybenzamide to give 2-[2-fluoro-3-methoxyphenyl]-6-methoxy- 5-(2-methylpropyl)-3-(2-phenylethyl)-4(3H)-pyrimidinone, which underwent demethylation to give compound II. All the invention compds. were evaluated for their calcium receptor inhibitory activity.

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

ST pyrimidinone prepn calcium receptor inhibitor treatment bone mineral disease

IT Proteins
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(ATPase inhibitor proteins, V-H+; preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)

IT Bone, disease
(Paget's, treatment of; preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)

IT Bone, disease
(abnormal, treatment of; preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)

IT Vitronectin receptors
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(antagonists; preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)

IT Gene, animal
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(c-src, SH2 antagonists; preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)

IT Bone, disease

(fracture, healing, treatment of; preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)

IT Neoplasm
(humoral hypercalcemia of malignancy, treatment of; preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)

IT Calcium-sensing receptors
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(inhibitors; preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)

IT Homeostasis
(mineral, treatment of; preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)

IT Bone, neoplasm
Sarcoma
(osteosarcoma, treatment of; preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)

IT Antiestrogens
Antiosteoporotic agents
Antirheumatic agents
Antitumor agents
Bone resorption inhibitors
(preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)

IT Calcium-sensing receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)

IT Estrogens
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)

IT Bone, disease
Neoplasm
Osteoarthritis
Osteoporosis
Periodontium, disease
Rheumatoid arthritis
(treatment of; preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)

IT 938181-19-2P
RL: BYP (Byproduct); PREP (Preparation)
(byproduct; preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)

IT 938177-13-0P 938177-15-2P 938177-17-4P 938177-24-3P 938177-37-8P
938177-39-0P 938178-22-4P 938178-61-1P 938178-70-2P 938179-64-7P
938179-78-3P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate and intermediate; preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone

and mineral diseases)

IT 938178-47-3P 938179-15-8P 938179-98-7P 938180-00-8P 938180-13-3P
938180-14-4P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(drug candidate; preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)

IT 780771-55-3P 938177-01-6P 938177-02-7P 938177-03-8P 938177-04-9P
938177-05-0P 938177-06-1P 938177-07-2P 938177-09-4P 938177-11-8P
938177-12-9P 938177-14-1P 938177-18-5P 938177-19-6P 938177-20-9P
938177-21-0P 938177-22-1P 938177-25-4P 938177-27-6P 938177-29-8P
938177-31-2P 938177-33-4P 938177-35-6P 938177-41-4P 938177-43-6P
938177-45-8P 938177-47-0P 938177-48-1P 938177-50-5P 938177-52-7P
938177-54-9P 938177-56-1P 938177-57-2P 938177-58-3P 938177-61-8P
938177-63-0P 938177-65-2P 938177-66-3P 938177-68-5P 938177-71-0P
938177-73-2P 938177-75-4P 938177-76-5P 938177-78-7P 938177-80-1P
938177-82-3P 938177-84-5P 938177-85-6P 938177-86-7P 938177-88-9P
938177-90-3P 938177-91-4P 938177-92-5P 938177-93-6P 938177-95-8P
938177-97-0P 938177-98-1P 938178-00-8P 938178-01-9P 938178-05-3P
938178-07-5P 938178-09-7P 938178-11-1P 938178-13-3P 938178-14-4P
938178-15-5P 938178-17-7P 938178-19-9P 938178-20-2P 938178-23-5P
938178-24-6P 938178-25-7P 938178-26-8P 938178-27-9P 938178-28-0P
938178-29-1P 938178-30-4P 938178-31-5P 938178-32-6P 938178-33-7P
938178-34-8P 938178-35-9P 938178-36-0P 938178-37-1P 938178-38-2P
938178-39-3P 938178-40-6P 938178-41-7P 938178-42-8P 938178-43-9P
938178-44-0P 938178-45-1P 938178-46-2P 938178-48-4P 938178-49-5P
938178-50-8P 938178-51-9P 938178-52-0P 938178-53-1P 938178-54-2P
938178-55-3P 938178-56-4P 938178-57-5P 938178-58-6P 938178-59-7P
938178-60-0P 938178-62-2P 938178-63-3P 938178-64-4P 938178-65-5P
938178-66-6P 938178-67-7P 938178-68-8P 938178-69-9P 938178-71-3P
938178-72-4P 938178-73-5P 938178-74-6P 938178-75-7P 938178-76-8P
938178-77-9P 938178-78-0P 938178-79-1P 938178-80-4P 938178-81-5P
938178-82-6P 938178-83-7P 938178-84-8P 938178-85-9P 938178-86-0P
938178-87-1P 938178-88-2P 938178-89-3P 938178-90-6P 938178-91-7P
938178-92-8P 938178-93-9P 938178-94-0P 938178-95-1P 938178-96-2P
938178-97-3P 938178-98-4P 938178-99-5P 938179-00-1P 938179-01-2P
938179-02-3P 938179-05-6P 938179-06-7P 938179-07-8P 938179-08-9P
938179-09-0P 938179-10-3P 938179-11-4P 938179-12-5P 938179-13-6P
938179-14-7P 938179-16-9P 938179-17-0P 938179-18-1P 938179-19-2P
938179-20-5P 938179-21-6P 938179-22-7P 938179-23-8P 938179-24-9P
938179-25-0P 938179-26-1P 938179-27-2P 938179-28-3P 938179-29-4P
938179-30-7P 938179-31-8P 938179-32-9P 938179-33-0P 938179-34-1P
938179-35-2P 938179-36-3P 938179-37-4P 938179-38-5P 938179-39-6P
938179-40-9P 938179-41-0P 938179-42-1P 938179-43-2P 938179-44-3P
938179-45-4P 938179-46-5P 938179-47-6P 938179-48-7P 938179-49-8P
938179-50-1P 938179-51-2P 938179-52-3P 938179-53-4P 938179-54-5P
938179-55-6P 938179-56-7P 938179-57-8P 938179-58-9P 938179-59-0P
938179-60-3P 938179-61-4P 938179-62-5P 938179-63-6P 938179-65-8P
938179-66-9P 938179-67-0P 938179-68-1P 938179-69-2P 938179-70-5P
938179-71-6P 938179-72-7P 938179-73-8P 938179-74-9P 938179-75-0P
938179-76-1P 938179-77-2P 938179-79-4P 938179-80-7P 938179-81-8P
938179-82-9P 938179-83-0P 938179-84-1P 938179-85-2P 938179-86-3P
938179-87-4P 938179-88-5P 938179-89-6P 938179-90-9P 938179-91-0P
938179-92-1P 938179-93-2P 938179-94-3P 938179-95-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of pyrimidinone derivs. as calcium

receptor inhibitors useful in the treatment of bone and mineral diseases)

IT 938179-96-5P 938179-97-6P 938179-99-8P 938180-01-9P 938180-02-0P 938180-03-1P 938180-04-2P 938180-05-3P 938180-06-4P 938180-07-5P 938180-08-6P 938180-09-7P 938180-10-0P 938180-11-1P 938180-12-2P 938180-15-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)

IT 94716-09-3, Cathepsin K
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(inhibitors; preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)

IT 1522-30-1P, Ethyl 2-acetyl-5-methylhexanoate 1540-31-4P, Ethyl 2-acetyl-3-methylpentanoate 2044-66-8P, 3-Oxo-N-(2-phenylethyl)butanamide 4116-18-1P, Ethyl 2-acetyl-3,3-dimethylbutanoate 4746-93-4P 20962-70-3P, Ethyl 2-acetyl-4-methyl-4-pentenoate 20962-71-4P, Methyl 2-acetyl-4-methyl-4-pentenoate 27773-10-0P, Ethyl 2-(2-methyl-1,3-dioxolan-2-yl)butanoate 50798-55-5P 51756-09-3P, Methyl 2-acetyl-4-methylpentanoate 51818-19-0P, 2-(Methoxy)benzenecarboximidamide 59698-18-9P, Phenylmethyl cyclopropylacetate 223418-75-5P, 2-Methyl-5-(tributylstannanyl)-1,3-thiazole 557101-33-4P, Ethyl 2-(cyclopropylmethyl)-3-oxobutanoate 705949-54-8P, 3-Fluoro-2-hydroxybenzamide 751428-10-1P, 2-(2-Methyl-1,3-dioxolan-2-yl)butanoic acid 854133-17-8P, N-[2-(3-Fluorophenyl)ethyl]-1,4-dioxaspiro[4.5]decane-6-carboxamide 854133-22-5P, 2-Ethyl-3-oxo-N-(2-phenylethyl)butanamide 854133-27-0P 854133-38-3P 874830-59-8P, 3-Fluoro-2-methoxybenzamide 938180-16-6P, 2-Acetyl-4-methyl-N-(2-phenylethyl)-4-pentenamide 938180-17-7P 938180-18-8P, N-[2-(3-Fluorophenyl)ethyl]-2-(2-methyl-1,3-dioxolan-2-yl)butanamide 938180-19-9P, 2-Ethyl-N-[2-(3-fluorophenyl)ethyl]-3-oxobutanamide 938180-20-2P 938180-21-3P 938180-22-4P 938180-23-5P 938180-24-6P 938180-25-7P 938180-26-8P 938180-27-9P 938180-28-0P 938180-29-1P 938180-30-4P 938180-31-5P 938180-32-6P 938180-33-7P 938180-34-8P 938180-35-9P, 3-Fluoro-2-[(phenylmethyl)oxy]benzonitrile 938180-36-0P 938180-37-1P 938180-38-2P 938180-39-3P 938180-40-6P 938180-41-7P, (2Z)-3-Amino-2-ethyl-N-[2-(3-fluorophenyl)ethyl]-2-butenamide 938180-42-8P 938180-43-9P 938180-44-0P, 3-Fluoro-2-(methoxy)benzenecarboximidamide 938180-45-1P 938180-46-2P 938180-47-3P 938180-48-4P 938180-49-5P 938180-50-8P 938180-51-9P 938180-52-0P 938180-53-1P 938180-54-2P 938180-55-3P 938180-56-4P 938180-57-5P 938180-58-6P 938180-59-7P 938180-60-0P 938180-61-1P 938180-62-2P 938180-63-3P 938180-64-4P 938180-65-5P 938180-66-6P 938180-67-7P 938180-68-8P 938180-69-9P 938180-70-2P 938180-71-3P 938180-72-4P 938180-73-5P, 4-[5-(Trimethylstannanyl)-2-thienyl]-1,3-oxazole 938180-74-6P 938180-75-7P, 2-(Cyclopropylmethyl)-3-oxo-N-(2-phenylethyl)butanamide 938180-76-8P, Phenylmethyl 2-cyclopropyl-3-oxobutanoate 938180-77-9P, 2-Cyclopropyl-3-oxo-N-(2-phenylethyl)butanamide 938180-78-0P, 2-Acetyl-N-[2-(3-fluorophenyl)ethyl]-5-methylhexanamide 938180-79-1P 938180-80-4P 938180-81-5P 938180-82-6P 938180-83-7P 938180-84-8P 938180-85-9P 938180-86-0P 938180-87-1P 938180-88-2P 938180-89-3P 938180-90-6P 938180-91-7P 938180-92-8P 938180-93-9P 938180-94-0P 938180-95-1P 938180-96-2P 938180-97-3P 938180-98-4P 938180-99-5P 938181-00-1P 938181-01-2P 938181-02-3P 938181-03-4P 938181-04-5P 938181-05-6P,

2-(2-Furanyl)-5,6,7,8-tetrahydro-4H-3,1-benzoxazin-4-one 938181-06-7P 938181-07-8P 938181-08-9P 938181-09-0P 938181-10-3P 938181-11-4P 938181-12-5P 938181-13-6P 938181-14-7P 938181-15-8P, 2-Acetyl-3-methyl-N-[2-(2-thienyl)ethyl]pentanamide 938181-16-9P 938181-17-0P 938181-18-1P 938181-20-5P 938181-21-6P 938181-22-7P 938181-23-8P 938181-24-9P 938181-25-0P 938181-26-1P 938181-27-2P, 2-Ethyl-3-oxo-N-(2-(thiophen-2-yl)ethyl)butanamide 938181-28-3P, 2-(2-Methyl-1,3-dioxolan-2-yl)-N-[2-(thienyl)ethyl]butanamide 938181-29-4P, (2Z)-3-Amino-2-ethyl-N-[2-(2-thienyl)ethyl]-2-butenamide 938181-30-7P 938181-31-8P 938181-32-9P, Ethyl 5-oxo-oxepane-4-carboxylate 938181-33-0P 938181-34-1P 938181-35-2P 938181-36-3P 938181-37-4P 938181-38-5P 938181-39-6P 938181-40-9P, N-[2-(3-Fluorophenyl)ethyl]-1-methyl-5-nitro-1H-pyrazole-4-carboxamide 938181-41-0P, 5-Amino-N-[2-(3-fluorophenyl)ethyl]-1-methyl-1H-pyrazole-4-carboxamide 938181-42-1P 938181-43-2P 938181-44-3P 938181-45-4P 938181-47-6P 938181-48-7P 938181-49-8P 938181-50-1P 938181-51-2P 938181-52-3P 938181-53-4P 938181-54-5P 938181-55-6P 938181-56-7P 938181-57-8P 938181-58-9P, 2-Acetyl-4-methyl-N-[2-(1-piperidinyl)ethyl]pentanamide 938181-59-0P 938181-60-3P 938181-61-4P 938181-62-5P 938181-63-6P 938181-64-7P 938181-65-8P, Methyl (2Z)-3-[([2-[(phenylmethyl)oxy]phenyl]carbonyl)amino]-2-butenoate 938181-66-9P 938181-67-0P 938181-68-1P 938181-69-2P 938181-70-5P 938181-71-6P 938181-72-7P 938181-73-8P, Phenylmethyl 3-fluoro-2-[(phenylmethyl)oxy]benzoate 938181-74-9P, 3-Fluoro-2-[(phenylmethyl)oxy]benzoic acid 938181-75-0P, 3-Fluoro-2-[(phenylmethyl)oxy]benzamide 938181-76-1P 938181-77-2P 938181-78-3P 938181-79-4P 938181-80-7P 938181-81-8P 938181-82-9P 938181-93-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)

IT 9007-12-9, Calcitonin 32222-06-3, 1α,25-(OH)2D3 41294-56-8, 1α-(OH)D3
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)

IT 938181-89-6P
RL: BYP (Byproduct); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(starting material; preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)

IT 55-21-0, Benzamide 62-53-3, Aniline, reactions 64-04-0, Phenethylamine 65-45-2, 2-Hydroxybenzamide 67-63-0, Isopropylalcohol, reactions 75-26-3, Isopropyl bromide 78-77-3, 1-Bromo-2-methylpropane 79-30-1, 2-Methylpropanoyl chloride 98-80-6, Phenylboronic acid 100-39-0, Benzyl bromide 103-63-9, 2-Bromoethylbenzene 105-45-3, Methyl acetoacetate 106-94-5, Propyl bromide 106-95-6, Allyl bromide, reactions 107-82-4, 1-Bromo-3-methylbutane 107-91-5, Cyanoacetamide 110-89-4, Piperidine, reactions 110-91-8, Morpholine, reactions 111-24-0, 1,5-Dibromopentane 123-75-1, Pyrrolidine, reactions 141-97-9, Ethyl 3-oxobutanoate 332-42-3, 1-(2-Bromoethyl)-4-fluorobenzene 341-27-5, 3-Fluoro-2-hydroxybenzoic acid 404-70-6, [2-(3-Fluorophenyl)ethyl]amine 445-28-3, 2-Fluorobenzamide 503-29-7, Azetidine 527-69-5, 2-Furancarbonyl chloride 541-41-3, Ethyl chloroformate 543-27-1, Isobutyl chloroformate 588-72-7, (E)-[2-Bromoethenyl]benzene 607-97-6, Ethyl 2-ethylacetoacetate

609-15-4, Ethyl 2-chloro-3-oxobutanoate 609-38-1, 2-Furancarboxamide 625-43-4, Methyl(2-methylpropyl)amine 661-69-8, Hexamethyldistannane 674-82-8 768-35-4, 3-Fluorophenylboronic acid 774-05-0, Ethyl 2-oxocycloheptanoate 960-16-7, Tributylphenyltin 1013-88-3, 1,1-Diphenylmethaneimine 1128-00-3 1423-26-3, 3-Trifluoromethylphenylboronic acid 1452-77-3, 2-Pyridinecarboxamide 1454-53-1, 1-Benzyl-4-oxopiperidine-3-carboxylic acid ethyl ester hydrochloride 1458-98-6, 3-Bromo-2-methyl-1-propene 1461-22-9, Tributyltin chloride 1468-39-9, 3-Methylbutanoic anhydride 1521-39-7, 2,3-Dimethoxybenzamide 1522-34-5, Ethyl 2-acetyl-4-methylpentanoate 1522-41-4, Ethyl 2-fluoro-3-oxo-butanoate 1522-46-9, Ethyl 2-acetyl-3-methylbutanoate 1540-29-0, Ethyl 2-acetylhexanoate 1540-32-5 1643-77-2, 4-Fluoro-2-hydroxybenzamide 1647-26-3, 2-Cyclohexylethyl bromide 1655-07-8, Ethyl 2-oxocyclohexanecarboxylate 1692-25-7, 3-Pyridinylboronic acid 1993-03-9, 2-Fluorophenylboronic acid 1997-80-4, 3-Trifluoromethylphenethyl bromide 2040-90-6, 2-Chloro-6-fluorophenol 2208-07-3, Ethyl acetimidate hydrochloride 2550-36-9, Cyclohexylmethyl bromide 2859-78-1, 3,4-Dimethoxyphenyl bromide 2873-18-9, 2-Chloro-5-bromothiophene 2975-41-9, 2,3-Dihydro-1H-inden-2-ylamine 3282-30-2, Pivaloyl chloride 3581-87-1, 2-Methylthiazole 3587-60-8, Chloromethyl phenylmethyl ether 4017-56-5, Ethyl 2-oxocyclooctanecarboxylate 4349-62-6, 2-Benzyloxybenzoyl chloride 4551-72-8, 1H-Pyrrole-2-carboxamide 4677-20-7, 4-(2-Bromoethyl)tetrahydro-2H-pyran 4743-87-7, 2-Acetylpent-4-enoic acid 5122-94-1, 4-Biphenylboronic acid 5239-82-7, Cyclopropylacetic acid 5271-67-0, 2-Thiophenecarbonyl chloride 5413-05-8, Ethyl 3-oxo-2-phenylbutanoate 5538-51-2, Acetic acid 2-chlorocarbonyl phenyl ester 5813-86-5, 3-Methoxybenzamide 5813-89-8, 2-Thiophenecarboxamide 5870-68-8, Ethyl 3-methylpentanoate 6165-69-1, Thiophene-3-boronic acid 6609-56-9, 2-Methoxybenzonitrile 7051-34-5, Bromomethylcyclopropane 7597-56-0 13331-27-6, 3-Nitrophenylboronic acid 14205-39-1, Methyl 3-aminocrotonate 14389-86-7, 2-Benzyloxybenzoic acid 14559-88-7 16093-82-6, Imidazole-2-carboxamide 16793-91-2, 2-Chlorophenethyl bromide 16799-05-6, 3-Chlorophenethyl bromide 17151-47-2 17247-58-4, Cyclobutylmethyl bromide 17376-04-4, 2-Iodoethylbenzene 18213-77-9, 1-Methyl-5-nitro-1H-pyrazole-4-carboxylic acid 18880-04-1, 3,4-Dichlorobenzyl bromide 18928-94-4, 2-Cyclopentylethyl bromide 21731-17-9, Methyl (2Z)-3-amino-2-butenoate 22237-13-4, 4-Ethoxyphenylboronic acid 24317-94-0, Ethyl 2-acetylheptanoate 25017-13-4, 1-(2-Bromoethyl)-3-fluorobenzene 26478-16-0, 2-(2-Bromoethyl)thiophene 27578-60-5, N-(2-Aminoethyl)piperidine 28611-39-4, 4-(N,N-Dimethylamino)phenylboronic acid 29214-60-6, Ethyl 2-acetyloctanoate 29943-42-8, Tetrahydropyran-4-one 30433-91-1, [2-(2-Thienyl)ethyl]amine 36239-09-5, Ethyl malonyl chloride 41051-15-4, Methyl 4-methoxy-3-oxobutanoate 52721-69-4, 2-Fluorophenethylamine 52784-32-4, Methyl 2-oxo-cycloheptanecarboxylate 53715-67-6, 5-Bromo-2-phenylthiazole 54663-78-4, Tributyl(2-thienyl)stannane 55552-70-0, 3-Furanboronic acid 57075-96-4 68971-88-0 71135-95-0, Methyl 2,2-dimethyl-6-oxocyclohexanecarboxylate 84110-40-7, 2-Methylpropylboronic acid 87199-15-3, 3-Hydroxymethylphenylboronic acid 90555-66-1, 3-Ethoxyphenylboronic acid 91319-54-9, 1-(2-Bromoethyl)-2-fluorobenzene 94839-07-3, 3,4-Methylenedioxyphenylboronic acid 98437-23-1, Benzothien-2-ylboronic acid 98437-24-2, 2-Benzofuranboronic acid 105445-58-7, 2-Tributylstannylbenzothiazole 113893-08-6, Benzothiophene-3-boronic acid 118486-94-5, Tributyl(2-furanyl)stannane 121359-48-6 122019-53-8 123324-71-0, 4-tert-Butylphenylboronic acid 126747-14-6, 4-Cyanophenylboronic acid 128796-39-4, 4-Trifluoromethylbenzeneboronic acid 135884-31-0, N-Boc-pyrrole-2-boronic acid 138642-62-3, 2-Cyanophenylboronic acid 139301-27-2, 4-Trifluoromethoxybenzeneboronic

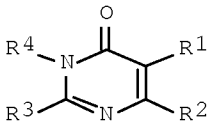
acid 141642-82-2 144025-03-6, 2,4-Difluorophenylboronic acid 146256-98-6 150255-96-2, 3-Cyanophenylboronic acid 153624-46-5, 4-Isopropoxyphenylboronic acid 156545-07-2, 3,5-Difluorophenylboronic acid 162607-15-0, 4-Methylthien-2-ylboronic acid 162607-20-7, 5-Methylthien-2-ylboronic acid 164014-95-3 168267-41-2, 3,4-Difluorophenylboronic acid 175203-60-8, 2-Bromo-5-chloro-3-methyl-benzothiophene 177735-09-0, 3-Methylthien-2-ylboronic acid 177735-30-7 191162-40-0 192182-55-1, N-Methylindole-5-boronic acid 198204-64-7, 2-Fluoro-3-methoxybenzamide 205371-27-3, 2-Tributylstannylpyrazine 206551-43-1, 5-Acetylthiophene-2-boronic acid 213211-69-9, 2-Ethoxyphenylboronic acid 251635-59-3, 4-Methyl-2-(tributylstannanyl)-1,3-thiazole 299426-80-5, Tributyl(5-methyl-3-thienyl)stannane 305832-67-1, (5-Cyanothien-2-yl)boronic acid 306934-95-2, 5-Phenylthien-2-ylboronic acid 321309-25-5, 5-(5-Bromo-2-thienyl)-1,3-oxazole 352018-87-2, 4-(5-Bromo-2-thienyl)-2-methyl-1,3-thiazole 373384-14-6, 3-(Dimethylcarbamoyl)phenylboronic acid 373384-18-0, 3-Methanesulfonylphenylboronic acid 376581-24-7, 6-Quinolinylboronic acid 438568-89-9, 2-Bromo-4,5,6,7-tetrahydro-1,3-benzothiazole 780771-63-3, 2-(Chlorocarbonyl)-6-fluorophenyl acetate 819849-22-4, [3-(N,N-Dimethylaminomethyl)phenyl]boronic acid 854133-23-6, 2-Ethyl-N-[2-(2-fluorophenyl)ethyl]-3-oxo-butanamide 938181-83-0 938181-84-1 938181-85-2 938181-86-3, 2-Cyclobutylmethyl-3-oxo-butyric acid ethyl ester 938181-87-4, 2-(2-Cyclohexylethyl)-3-oxo-butanoic acid 938181-88-5, Tributyl(4,5-dimethyl-2-thienyl)stannane 938181-90-9, 2-(5-Bromo-2-thienyl)-5-methyl-1,3,4-oxadiazole 938181-91-0, 5-Bromo-2-(2-hydroxyphenyl)-6-(methoxymethyl)-3-(2-phenylethyl)-4(3H)-pyrimidinone 938181-92-1, 4,5-Dimethyl-2-(tributylstannanyl)-1,3-thiazole
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)

L79 ANSWER 3 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 3
ACCESSION NUMBER: 2006:361302 ZCAPLUS Full-text
DOCUMENT NUMBER: 144:412524
TITLE: Preparation of reversed pyrimidinone compounds as calcilytics
INVENTOR(S): Marquis, Robert W.; Yamashita, Dennis Shinji; Jeong, Jae U.; Leungo, Juan I.
PATENT ASSIGNEE(S): Nps Pharmaceuticals, Inc., USA; Glaxosmithkline
SOURCE: PCT Int. Appl., 54 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006041968	A1	20060420	WO 2005-US35906	20051006

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,

CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TM
EP 1809611 A1 20070725 EP 2005-804245 20051006
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR
JP 2008515902 T 20080515 JP 2007-535792 20051006
US 20070270446 A1 20071122 US 2007-663238 20070727
PRIORITY APPLN. INFO.: US 2004-616389P P 20041006
WO 2005-US35906 W 20051006
OTHER SOURCE(S): CASREACT 144:412524; MARPAT 144:412524
GI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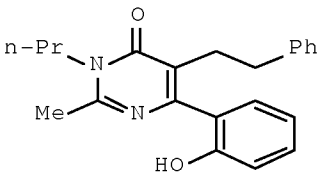

II

AB Title compds. I [wherein R1 = H, alkyl, aryl, etc.; R2 = (un)substituted aryl; R3, R4 = H, halo, alkyl, etc.; R3 and R4 may link together to form a ring] and pharmaceutically acceptable salts, hydrates, tautomers, solvates or complexes thereof, which are useful as inhibitors of calcium receptors in the treatment of diseases associated with abnormal bone or mineral homeostasis (no data), were prepared For instance, condensation of Me 4-phenylbutyrate with Me 2-methoxybenzoate using NaH as base gave a β-keto ester (75% yield), which underwent successive cyclization with acetamidine hydrochloride in the presence of NaOMe to a pyrimidinone (64% yield), N-alkylation with 1-bromopropane (59% yield) and demethylation with BBr3 (66% yield) to afford II.

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63
ST pyrimidinone prepn calcilytic homeostasis; calcium receptor inhibitor pyrimidinone prepn
IT Bone, disease
(Paget's; preparation of reversed pyrimidinone compds. as calcilytics)
IT Homeostasis
(abnormal bone or mineral; preparation of reversed pyrimidinone compds. as calcilytics)
IT Vitronectin receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(antagonists, compns. comprising; preparation of reversed pyrimidinone compds. as calcilytics)
IT Receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(calcium, inhibitor; preparation of reversed pyrimidinone compds. as calcilytics)
IT Bone resorption inhibitors
Diphosphonates
Selective estrogen receptor modulators
(compns. comprising; preparation of reversed pyrimidinone compds. as calcilytics)
IT Estrogens

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(compns. comprising; preparation of reversed pyrimidinone compds. as calcilytics)

IT Neoplasm
(humoral hypercalcemia of malignancy, treatment of; preparation of reversed pyrimidinone compds. as calcilytics)

IT Parathyroid gland
(increasing serum parathyroid levels; preparation of reversed pyrimidinone compds. as calcilytics)

IT Joint, anatomical
(joint replacement; preparation of reversed pyrimidinone compds. as calcilytics)

IT Bone, neoplasm
Sarcoma
(osteosarcoma, treatment of; preparation of reversed pyrimidinone compds. as calcilytics)

IT Antiosteoporotic agents
Antirheumatic agents
Antitumor agents
Bone resorption inhibitors
Combination chemotherapy
Human
Wound healing
(preparation of reversed pyrimidinone compds. as calcilytics)

IT Neoplasm
Osteoarthritis
Periodontium, disease
Rheumatoid arthritis
(treatment of; preparation of reversed pyrimidinone compds. as calcilytics)

IT 144697-17-6
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(antagonists, compns. comprising; preparation of reversed pyrimidinone compds. as calcilytics)

IT 9007-12-9, Calcitonin 66772-14-3, 1,25-Dihydroxyvitamin D
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(compns. comprising; preparation of reversed pyrimidinone compds. as calcilytics)

IT 883745-13-9P 883745-22-0P 883745-24-2P 883745-26-4P 883745-28-6P
883745-29-7P 883745-30-0P 883745-31-1P 883745-32-2P 883745-33-3P
883745-34-4P 883745-35-5P 883745-36-6P 883745-37-7P 883745-38-8P
883745-39-9P 883745-40-2P 883745-44-6P 883745-45-7P 883745-46-8P
883745-47-9P 883745-48-0P 883745-49-1P 883745-50-4P 883745-51-5P
883745-52-6P 883745-53-7P 883745-54-8P 883745-55-9P 883745-56-0P
883745-57-1P 883745-60-6P 883745-61-7P 883745-62-8P 883745-63-9P
883745-64-0P 883745-65-1P 883745-67-3P 883745-68-4P 883745-69-5P
883745-72-0P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of reversed pyrimidinone compds. as calcilytics)

IT 94716-09-3, Cathepsin K
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(inhibitors, compns. comprising; preparation of reversed pyrimidinone compds. as calcilytics)

IT 62-53-3, Aniline, reactions 75-31-0, 2-Propanamine, reactions 78-81-9, (2-Methylpropyl)amine 92-67-1, 4-Aminobiphenyl 106-94-5, 1-Bromopropane 106-95-6, Allyl bromide, reactions 107-82-4,

1-Bromo-3-methylbutane 108-91-8, Cyclohexanamine, reactions 109-65-9, 1-Bromobutane 110-53-2, 1-Bromopentane 111-25-1, 1-Bromohexane 143-37-3, Acetamidine 341-27-5, 3-Fluoro-2-hydroxybenzoic acid 542-69-8, 1-Iodobutane 606-45-1, Methyl 2-(methoxy)benzoate 629-04-9, 1-Bromoheptane 629-27-6, 1-Iodooctane 753-90-2 765-30-0, Cyclopropanamine 1003-03-8, Cyclopentanamine 1013-88-3, 1,1-Diphenylmethanimine 1186-46-5, 1,1-Dimethylguanidine sulfate 1458-98-6, 3-Bromo-2-methylprop-1-ene 1647-26-3, 1-Bromo-2-cyclohexylethane 2046-17-5, Methyl 4-phenylbutyrate 2516-34-9, Cyclobutanamine 5813-64-9, (2,2-Dimethylpropyl)amine 6314-28-9, Benzo[b]thiophene-2-carboxylic acid 7051-34-5, (Bromomethyl)cyclopropane 13952-84-6, 2-Butanamine 14770-82-2 15972-01-7 22780-54-7 29488-24-2, 2-Bromo-5-phenylthiophene 51387-90-7, [2-(1-Methyl-2-pyrrolidinyl)ethyl]amine 55401-97-3, 2-Bromomethylpyridine 55502-89-1, 2-Amino-5-methylthiophene 106428-05-1, 3-Fluoro-2-methoxybenzoic acid 883745-71-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of reversed pyrimidinone compds. as calcilytics)

IT 4521-30-6P, Benzo[b]thiophen-2-amine 14770-85-5P 89673-36-9P 106428-04-0P 883745-15-1P 883745-17-3P 883745-20-8P 883745-41-3P 883745-42-4P 883745-43-5P 883745-58-2P 883745-59-3P 883745-66-2P 883745-70-8P 883745-73-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of reversed pyrimidinone compds. as calcilytics)

IT 9000-83-3
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(proton-translocating, inhibitors, compns. comprising; preparation of reversed pyrimidinone compds. as calcilytics)

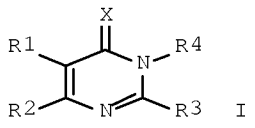
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 4 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 4
ACCESSION NUMBER: 2005:1215763 ZCAPLUS Full-text
DOCUMENT NUMBER: 143:477975
TITLE: Preparation of pyrimidinones and quinazolinones as calcilytic compounds
INVENTOR(S): Luengo, Juan I.; Marquis, Robert W., Jr.; Xie, Ren; Yamashita, Dennis S.
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA
SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005108376	A1	20051117	WO 2005-US15224	20050503

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,

AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT,
RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML,
MR, NE, SN, TD, TG
EP 1742924 A1 20070117 EP 2005-744198 20050503
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, HR, LV
JP 2007536239 T 20071213 JP 2007-511482 20050503
US 20070232628 A1 20071004 US 2006-568709 20061106
PRIORITY APPLN. INFO.: US 2004-568585P P 20040506
WO 2005-US15224 W 20050503
OTHER SOURCE(S): CASREACT 143:477975; MARPAT 143:477975
GI



I

AB The title compds. I [R1, R2 = H, halo, CN, etc.; or R1 and R2 may be bonded together to form a carbocyclic, heterocylic, aryl or heteroaryl ring; R3 = aryl or heteroaryl group which may have 1-5 substituents each selected from H, halo, CN, CF3, etc.; R4 = aryl which may have 1-3 substituents consisting of H, halo, CN, CF3, etc.; X = O or S], useful for treating a disease or disorder characterized by an abnormal bone or mineral homeostasis, were prepared E.g., a multi-step synthesis of 2-(2-hydroxyphenyl)-3-(4-isopropylphenyl)-5,6,7,8-tetrahydro-3H-quinazolin- 4-one, starting from Et 2-aminocyclohex-1-enecarboxylate and 2-benzyloxybenzoyl chloride, was given. The methods for treating diseases or disorders such as osteosarcoma, periodontal disease, fracture healing, osteoarthritis, joint replacement, rheumatoid arthritis, Paget's disease, humoral hypercalcemia, malignancy and osteoporosis by administering the compound I alone or in combination with anti-resorptive agents are disclosed.

IC ICM C07D239-36
ICS C07D239-91; A61K031-513; A61K031-517
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63
ST pyrimidinone prepn calcilytic calcium receptor antagonist bone disease treatment; quinazolinone prepn calcilytic calcium receptor antagonist bone disease treatment
IT Bone, disease
(Paget's, treating; preparation of pyrimidinones and quinazolinones as calcilytic compds.)
IT Disease, animal
(arthropathy, treating joint replacement; preparation of pyrimidinones and quinazolinones as calcilytic compds.)
IT Receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(calcium; preparation of pyrimidinones and quinazolinones as calcilytic compds.)
IT Estrogens
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(co-drug; preparation of pyrimidinones and quinazolinones as calcilytic compds.)

IT Joint, anatomical
(disease, treating joint replacement; preparation of pyrimidinones and quinazolinones as calcilytic compds.)

IT Bone, disease
(fracture, treating fracture healing; preparation of pyrimidinones and quinazolinones as calcilytic compds.)

IT Neoplasm
(humoral hypercalcemia of malignancy, treating; preparation of pyrimidinones and quinazolinones as calcilytic compds.)

IT Bone, neoplasm
Sarcoma
(osteosarcoma, treating; preparation of pyrimidinones and quinazolinones as calcilytic compds.)

IT Antirheumatic agents
Combination chemotherapy
Human
(preparation of pyrimidinones and quinazolinones as calcilytic compds.)

IT Parathyroid gland
(preparation of pyrimidinones and quinazolinones for increasing serum parathyroid levels)

IT Bone, neoplasm
Osteoarthritis
Osteoporosis
Periodontium, disease
Rheumatoid arthritis
(treating; preparation of pyrimidinones and quinazolinones as calcilytic compds.)

IT 9007-12-9, Calcitonin 32222-06-3
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(co-drug; preparation of pyrimidinones and quinazolinones as calcilytic compds.)

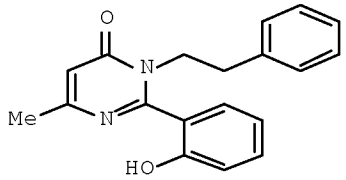
IT 869564-56-7P 869564-58-9P 869564-60-3P 869564-62-5P 869564-64-7P
869564-66-9P 869564-68-1P 869564-70-5P 869564-72-7P 869564-74-9P
869564-76-1P 869564-98-7P 869564-99-8P 869565-00-4P 869565-01-5P
869565-02-6P 869565-03-7P 869565-04-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidinones and quinazolinones as calcilytic compds.)

IT 65-45-2, Salicylamide 98-80-6, Phenylboronic acid 99-88-7, 4-Isopropylaniline 105-45-3, Methyl acetoacetate 607-97-6, Ethyl 2-ethyl-3-oxobutyrate 609-14-3, Ethyl 2-methylacetoacetate 610-89-9, Ethyl 2-acetyl-4-pentenoate 626-34-6 1128-00-3 1540-29-0, Ethyl 2-butylacetoacetate 4349-62-6, 2-Benzyloxybenzoyl chloride 21615-34-9, 2-Anisoyl chloride 98437-23-1 780771-63-3 869564-97-6 874830-59-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrimidinones and quinazolinones as calcilytic compds.)

IT 27773-10-0P 401639-34-7P 751428-10-1P 869564-78-3P 869564-80-7P
869564-82-9P 869564-83-0P 869564-84-1P 869564-86-3P 869564-87-4P
869564-88-5P 869564-89-6P 869564-90-9P 869564-91-0P 869564-92-1P
869564-93-2P 869564-94-3P 869564-95-4P 869564-96-5P 920264-52-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrimidinones and quinazolinones as

calcilytic compds.)
REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 5 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 5
ACCESSION NUMBER: 2005:378882 ZCAPLUS Full-text
DOCUMENT NUMBER: 143:59927
TITLE: Design, new synthesis, and calcilytic activity of substituted 3H-pyrimidin-4-ones
AUTHOR(S): Shcherbakova, Irina; Huang, Guangfei; Geoffroy, Otto J.; Nair, Satheesh K.; Swierczek, Krzysztof; Balandrin, Manuel F.; Fox, John; Heaton, William L.; Conklin, Rebecca L.
CORPORATE SOURCE: Drug Discovery, NPS Pharmaceuticals, Inc., Salt Lake City, UT, 84108, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(10), 2537-2540
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:59927
GI



I

AB Design, synthesis, structure-activity relationship studies and calcium receptor antagonist (calcilytic) properties of 3H-pyrimidin-4-ones, e.g., I, are described. The pyrimidinones were synthesized by multistep procedures.
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
ST keto ester amidine heterocyclization; pyrimidinone prepn calcilytic
IT Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(aralkyl; preparation, calcilytic activity, and structure-activity relationship of substituted pyrimidinones starting from hydroxybenzonitrile or β-keto esters and phenylethylamines using multistep procedures)
IT Receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(calcium; preparation, calcilytic activity, and structure-activity relationship of substituted pyrimidinones starting from hydroxybenzonitrile or β-keto esters and phenylethylamines using multistep procedures)
IT Carboxylic acids, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxo, esters; preparation, calcilytic activity, and

structure-activity relationship of substituted pyrimidinones starting from hydroxybenzonitrile or β-keto esters and phenylethylamines using multistep procedures)

IT Heterocyclization
(preparation, calcilytic activity, and structure-activity relationship of substituted pyrimidinones starting from hydroxybenzonitrile or β-keto esters and phenylethylamines using multistep procedures)

IT Structure-activity relationship
(receptor-binding, CaR; preparation, calcilytic activity, and structure-activity relationship of substituted pyrimidinones starting from hydroxybenzonitrile or β-keto esters and phenylethylamines using multistep procedures)

IT 780771-32-6P 780771-33-7P 780771-34-8P 780771-35-9P 780771-41-7P
780771-43-9P 780771-44-0P 780771-47-3P 780771-48-4P 780771-53-1P
780771-54-2P 780771-55-3P 780771-56-4P 780771-57-5P 780771-58-6P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation, calcilytic activity, and structure-activity relationship of substituted pyrimidinones starting from hydroxybenzonitrile or β-keto esters and phenylethylamines using multistep procedures)

IT 64-04-0, 2-Phenylethylamine 105-45-3, Methyl acetoacetate 344-00-3
404-70-6, 2-(3-Fluorophenyl)ethylamine 607-97-6 609-14-3 611-10-9
611-20-1, 2-Hydroxybenzonitrile 1522-46-9 1540-28-9 1655-07-8
5538-51-2, 2-Acetoxybenzoyl chloride 22396-14-1 52721-69-4,
2-(2-Fluorophenyl)ethylamine
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation, calcilytic activity, and structure-activity relationship of substituted pyrimidinones starting from hydroxybenzonitrile or β-keto esters and phenylethylamines using multistep procedures)

IT 4746-93-4P 7646-61-9P 13747-72-3P 23153-73-3P 26384-76-9P
27773-09-7P 27773-10-0P 38853-85-9P 85796-29-8P 90647-54-4P
130625-27-3P 610754-95-5P 751428-10-1P 780771-36-0P 780771-37-1P
780771-38-2P 780771-39-3P 854132-93-7P 854132-94-8P 854132-95-9P
854132-96-0P 854132-97-1P 854132-98-2P 854132-99-3P 854133-00-9P
854133-01-0P 854133-02-1P 854133-03-2P 854133-04-3P 854133-05-4P
854133-06-5P 854133-07-6P 854133-08-7P 854133-09-8P 854133-10-1P
854133-11-2P 854133-12-3P 854133-13-4P 854133-14-5P 854133-15-6P
854133-16-7P 854133-17-8P 854133-18-9P 854133-19-0P 854133-20-3P
854133-21-4P 854133-22-5P 854133-23-6P 854133-24-7P 854133-25-8P
854133-26-9P 854133-27-0P 854133-28-1P 854133-29-2P 854133-30-5P
854133-31-6P 854133-32-7P 854133-33-8P 854133-34-9P 854133-35-0P
854133-36-1P 854133-37-2P 854133-38-3P 854133-39-4P 854133-40-7P
854133-41-8P 854133-42-9P 854133-43-0P 854133-44-1P 854133-45-2P
854133-46-3P 854133-47-4P 854133-48-5P 854133-49-6P 854133-50-9P
854133-51-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, calcilytic activity, and structure-activity relationship of substituted pyrimidinones starting from hydroxybenzonitrile or β-keto esters and phenylethylamines using multistep procedures)

REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 6 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 6
ACCESSION NUMBER: 2005:199466 ZCAPLUS Full-text

DOCUMENT NUMBER: 142:348143
TITLE: 3H-Quinazolin-4-ones as a new calcilytic template for the potential treatment of osteoporosis
AUTHOR(S): Shcherbakova, Irina; Balandrin, Manuel F.; Fox, John; Ghatak, Anjan; Heaton, William L.; Conklin, Rebecca L.
CORPORATE SOURCE: Drug Discovery, NPS Pharmaceuticals, Inc., Salt Lake City, UT, 84108, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(6), 1557-1560
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 142:348143
AB Structure-activity relationship studies, focused on identification of the active pharmacophore fragments in a single high-throughput screening calcilytic hit, resulted in the discovery of potent calcium receptor antagonists, substituted 3H-quinazolin-4-ones.
CC 1-3 (Pharmacology)
Section cross-reference(s): 28
REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 7 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 7
ACCESSION NUMBER: 2004:902339 ZCAPLUS Full-text
DOCUMENT NUMBER: 141:379934
TITLE: Preparation of 2,3,5,6-tetrasubstituted 3H-pyrimidin-4-ones via cyclization of carboxamides.
INVENTOR(S): Shcherbakova, Irina; Balandrin, Manuel; Huang, Guangfei; Geoffroy, Otto; Fox, John; Nair, Satheesh K.
PATENT ASSIGNEE(S): NPS Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 33 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004092121	A2	20041028	WO 2004-US10639	20040407
WO 2004092121	A3	20050414		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1613606	A2	20060111	EP 2004-749815	20040407
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
JP 2006522160	T	20060928	JP 2006-509759	20040407
US 20070161792	A1	20070712	US 2006-551920	20061120
PRIORITY APPLN. INFO.:			US 2003-460859P P	20030407

	US 2003-479323P	P	20030618
	WO 2004-US10639	W	20040407

OTHER SOURCE(S): CASREACT 141:379934; MARPAT 141:379934

AB The title process is claimed. Thus, 3-(2-acetoxybenzoylamino)-2-methylbut- 2-enoic acid phenethylamide (preparation given) was refluxed overnight with KOH in EtOH/H2O to give 37% 2-(2-hydroxyphenyl)-5,6-dimethyl-3-phenethyl-3H-pyrimidin-4-one.

IC ICM C07D

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))

ST pyrimidinone tetrasubstituted prepn; cyclopentapyrimidinone quinazolinone prepn; aroylaminoacrylamide cyclization reaction; hydroxyphenyldimethylphenethylpyrimidinone prepn

IT Cyclization
(aroylaminoacrylamide cyclization reaction; preparation of tetrasubstituted pyrimidinones via cyclization of carboxamides)

IT 780771-35-9P 780771-40-6P 780771-41-7P 780771-42-8P 780771-43-9P 780771-44-0P 780771-45-1P 780771-46-2P 780771-47-3P 780771-48-4P 780771-51-9P 780771-52-0P 780771-54-2P 780771-55-3P 780771-56-4P 780771-57-5P 780771-58-6P 916335-88-1P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of tetrasubstituted pyrimidinones via cyclization of carboxamides)

IT 64-04-0, Phenethylamine 404-70-6, 3-Fluorophenethylamine 607-97-6, Ethyl 2-ethyl-3-oxobutyrate 609-14-3, Ethyl 2-methyl-3-oxobutyrate 611-10-9, Ethyl 2-oxocyclopentanecarboxylate 1583-88-6, 4-Fluorophenethylamine 1655-07-8, Ethyl 2-oxocyclohexanecarboxylate 5538-51-2 21615-34-9 22396-14-1 51756-10-6 52721-69-4, 2-Fluorophenethylamine 116046-53-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of tetrasubstituted pyrimidinones via cyclization of carboxamides)

IT 85796-29-8P 128095-14-7P 780771-36-0P 780771-37-1P 780771-38-2P 780771-39-3P 780771-49-5P, 3-Amino-2-isopropylbut-3-enoic acid methyl ester 780771-50-8P, 2-Isopropyl-3-(2-methoxybenzoylamino)but-3-enoic acid methyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of tetrasubstituted pyrimidinones via cyclization of carboxamides)

L79 ANSWER 8 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 8

ACCESSION NUMBER: 2004:902338 ZCAPLUS Full-text

DOCUMENT NUMBER: 141:366249

TITLE: Preparation of pyrimidinone compounds as calcilytics

INVENTOR(S): Shcherbakova, Irina V.; Balandrin, Manuel F.; Huang, Guangfei; Geoffroy, Otto; Fox, John; Marquis, Robert; Yamashita, Dennis Shinji; Luengo, Juan; Wang, Wenyong

PATENT ASSIGNEE(S): NPS Pharmaceuticals, Inc., USA; Glaxosmithkline

SOURCE: PCT Int. Appl., 57 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004092120	A2	20041028	WO 2004-US10638	20040407

WO 2004092120 A3 20050414
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2004230903	A1	20041028	AU 2004-230903		20040407
CA 2521129	A1	20041028	CA 2004-2521129		20040407
EP 1615897	A2	20060118	EP 2004-749814		20040407
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR					
CN 1835928	A	20060920	CN 2004-80009255		20040407
JP 2006522159	T	20060928	JP 2006-509758		20040407
MX 2005PA10683	A	20060801	MX 2005-PA10683		20051004
US 20070197555	A1	20070823	US 2006-552363		20061120
PRIORITY APPLN. INFO.:			US 2003-460859P	P	20030407
			US 2003-479323P	P	20030618
			WO 2004-US10638	W	20040407

OTHER SOURCE(S): CASREACT 141:366249; MARPAT 141:366249

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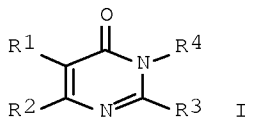


I

AB Title compds. I [R1-2 = H, halo, CN, CF3, etc.; R3 = aryl; R4 = H, alkyl, etc.] are prepared For instance, 2-(2-Hydroxyphenyl)-6-methyl-3-phenethyl-3H-pyrimidin-4-one is prepared from o-hydroxybenzonitrile, acetyl chloride and Me acetoacetate. Compds. of the invention have IC50 values < 30 μM in a calcium receptor inhibition assay. I are useful for the treatment of abnormal bone or mineral homeostasis.

IC ICM C07D
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63
ST pyrimidinone calcilytic calcium receptor antagonist prepn
IT Bone, disease
(Paget's; preparation of pyrimidinone compds. as calcilytics)
IT Homeostasis
(bone or mineral disorders; preparation of pyrimidinone compds. as calcilytics)
IT Receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(calcium; preparation of pyrimidinone compds. as calcilytics)
IT Bone, neoplasm
Sarcoma

(osteosarcoma; preparation of pyrimidinone compds. as calcilytics)

IT Antirheumatic agents
Human
Osteoarthritis
Osteoporosis
Periodontium, disease
Rheumatoid arthritis
Wound healing
(preparation of pyrimidinone compds. as calcilytics)

IT 7440-70-2, Calcium, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(hypercalcemia; preparation of pyrimidinone compds. as calcilytics)

IT 9002-64-6, Parathyroid hormone
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of pyrimidinone compds. as calcilytics)

IT 780771-43-9P, 5-Ethyl-2-(2-hydroxyphenyl)-6-methyl-3-phenethyl-3H-pyrimidin-4-one 780771-51-9P, 3-[2-(3-Fluorophenyl)ethyl]-5-isopropyl-2-(2-methoxyphenyl)-6-methyl-3H-pyrimidin-4-one
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of pyrimidinone compds. as calcilytics)

IT 780771-32-6P, 2-(2-Hydroxyphenyl)-6-methyl-3-phenethyl-3H-pyrimidin-4-one 780771-33-7P, 3-[2-(2-Fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-3H-pyrimidin-4-one 780771-34-8P, 3-[2-(3-Fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-3H-pyrimidin-4-one 780771-35-9P, 2-(2-Hydroxyphenyl)-5,6-dimethyl-3-phenethyl-3H-pyrimidin-4-one 780771-40-6P, 3-[2-(2-Fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5,6-dimethyl-3H-pyrimidin-4-one 780771-41-7P, 3-[2-(3-Fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5,6-dimethyl-3H-pyrimidin-4-one 780771-42-8P, 3-[2-(4-Fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5,6-dimethyl-3H-pyrimidin-4-one 780771-44-0P, 5-Ethyl-3-[2-(2-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-3H-pyrimidin-4-one 780771-45-1P 780771-46-2P, 5-Ethyl-3-[2-(4-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-3H-pyrimidin-4-one 780771-47-3P, 3-[2-(3-Fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-5-propyl-3H-pyrimidin-4-one 780771-48-4P, 3-[2-(3-Fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5-isopropyl-6-methyl-3H-pyrimidin-4-one 780771-52-0P, 3-[2-(2-Fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5-isopropyl-6-methyl-3H-pyrimidin-4-one 780771-53-1P, 2-(2-Hydroxyphenyl)-5-methyl-3-phenethyl-6-trifluoromethyl-3H-pyrimidin-4-one 780771-54-2P, 2-(2-Hydroxyphenyl)-3-phenethyl-5,6,7,8-tetrahydro-3H-quinazolin-4-one 780771-55-3P, 3-[2-(3-Fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5,6,7,8-tetrahydro-3H-quinazolin-4-one 780771-56-4P, 5-Cyclopropyl-3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-3H-pyrimidin-4-one 780771-57-5P, 2-(2-Hydroxyphenyl)-3-phenethyl-3,5,6,7-tetrahydrocyclopenta[1,2-d]pyrimidin-4-one 780771-58-6P, 3-[2-(3-Fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-3,5,6,7-tetrahydrocyclopenta[1,2-d]pyrimidin-4-one 780771-59-7P, 5-Ethyl-2-(2-methoxyphenyl)-6-methyl-3-phenethyl-3H-pyrimidin-4-one 780771-60-0P, 2-(5-Chloro-2-hydroxypyridin-3-yl)-5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl-3H-pyrimidin-4-one 780771-62-2P, 5-Ethyl-2-(3-fluoro-2-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl-3H-pyrimidin-4-one 780771-64-4P, 5-Ethyl-2-(5-fluoro-2-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl-3H-pyrimidin-4-one 780771-65-5P, 5-Ethyl-2-(2-fluoro-6-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl-3H-pyrimidin-4-one 780771-67-7P, 2-(5-Chloro-2-hydroxyphenyl)-5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl-3H-pyrimidin-4-one 780771-68-8P, 2-(5-Bromo-2-hydroxyphenyl)-5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl-

3H-pyrimidin-4-one 780771-69-9P, 5-Ethyl-3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxy-3-isopropylphenyl)-6-methyl-3H-pyrimidin-4-one 780771-71-3P, 2-(3,5-Dibromo-2-hydroxyphenyl)-5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl-3H-pyrimidin-4-one 780771-72-4P, 5-Ethyl-2-(3-chloro-2-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl-3H-pyrimidin-4-one 780771-74-6P, 5-Ethyl-3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxy-3-methylphenyl)-6-methyl-3H-pyrimidin-4-one 780771-75-7P, 2-(4-Chloro-2-hydroxyphenyl)-5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl-3H-pyrimidin-4-one 780771-76-8P, 5-Ethyl-3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxy-4-methoxyphenyl)-6-methyl-3H-pyrimidin-4-one
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidinone compds. as calcilytics)

IT 64-04-0, Phenethylamine 75-36-5, Acetyl chloride 100-58-3, Phenylmagnesium bromide 105-45-3, Methyl acetoacetate 404-70-6, 2-(3-Fluorophenyl)ethylamine 607-97-6, 2-Ethyl-3-oxobutanoic acid ethyl ester 609-14-3, 2-Methyl-3-oxobutyric acid ethyl ester 611-10-9, 2-Oxocyclopentanecarboxylic acid ethyl ester 611-20-1, o-Hydroxybenzonitrile 1522-46-9, 2-Isopropyl-3-oxobutanoic acid ethyl ester 1540-28-9, 2-Propyl-3-oxobutanoic acid ethyl ester 1583-88-6, 4-Fluorophenethylamine 1655-07-8, 2-Oxocyclohexanecarboxylic acid ethyl ester 5485-91-6, Acetic acid 4-bromo-2-chlorocarbonylphenyl ester 5538-51-2, Acetic acid 2-chlorocarbonylphenyl ester 5538-52-3, Acetic acid 2-chlorocarbonyl-4-fluorophenyl ester 5538-53-4, Acetic acid 4-chloro-2-chlorocarbonylphenyl ester 17094-21-2, 2-Methyl-3-oxobutanoic acid methyl ester 19202-27-8, Acetic acid 2-chlorocarbonylmethoxyphenyl ester 21615-34-9 22396-14-1, 2-Cyclopropyl-3-oxobutanoic acid ethyl ester 26384-76-9 27893-05-6, Acetic acid 2-chlorocarbonyl-6-methylphenyl ester 52721-69-4, 2-(2-Fluorophenyl)ethylamine 54223-78-8 54551-50-7, Acetic acid 5-chloro-2-chlorocarbonylphenyl ester 116046-53-8, 2-Trifluoromethyl-3-oxobutanoic acid ethyl ester 780771-61-1, 2-Acetoxy-5-chloronicotinoyl chloride 780771-63-3, Acetic acid 2-chlorocarbonyl-6-fluorophenyl ester 780771-66-6, Acetic acid 2-chlorocarbonyl-3-fluorophenyl ester 780771-70-2, Acetic acid 2-chlorocarbonyl-6-isopropylphenyl ester 780771-73-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrimidinone compds. as calcilytics)

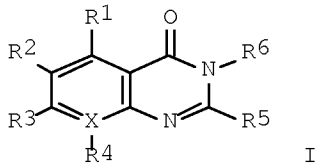
IT 27773-09-7P, 2-(2-Methyl-[1,3]dioxolan-2-yl)propionic acid ethyl ester 61636-46-2P 85796-29-8P, 2-(2-Methyl-[1,3]dioxolan-2-yl)propionic acid 780771-36-0P, 2-(2-Methyl-[1,3]dioxolan-2-yl)-N-phenethylpropaneamide 780771-37-1P, 2-Methyl-3-oxo-N-phenethylbutyramide 780771-38-2P, 3-Amino-2-methylbut-2-enoic acid phenethylamide 780771-39-3P, Acetic acid 2-((1-methyl-2-((phenethyl)carbamoyl)propenyl)carbamoyl)phenyl ester 780771-49-5P, 3-Amino-2-isopropylbut-3-enoic acid methyl ester 780771-50-8P, 2-Isopropyl-3-(2-methoxybenzoylamino)but-3-enoic acid methyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrimidinone compds. as calcilytics)

L79 ANSWER 9 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 9
ACCESSION NUMBER: 2004:412903 ZCAPLUS Full-text
DOCUMENT NUMBER: 140:423688
TITLE: Preparation of quinazolinone derivatives as calcilytics
INVENTOR(S): Shcherbakova, Irina; Balandrin, Manuel; Fox, John; Heaton, William; Conklin, Rebecca; Papac, Damon
PATENT ASSIGNEE(S): NPS Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 74 pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2004041755	A2	20040521	WO 2003-US35162		20031104
WO 2004041755	A3	20040708			
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
CA 2502302	A1	20040521	CA 2003-2502302		20031104
AU 2003291761	A1	20040607	AU 2003-291761		20031104
EP 1558260	A2	20050803	EP 2003-768655		20031104
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
CN 1708306	A	20051214	CN 2003-80102626		20031104
JP 2006512315	T	20060413	JP 2004-550482		20031104
US 20060052345	A1	20060309	US 2005-531161		20050412
MX 2005PA04328	A	20050802	MX 2005-PA4328		20050422
PRIORITY APPLN. INFO.:			US 2002-423663P	P	20021104
			WO 2003-US35162	W	20031104

OTHER SOURCE(S): MARPAT 140:423688
GI



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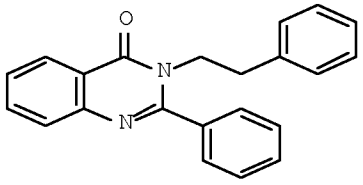


II

AB The title compds. I [R1, R2, R3 = H, halo, CN, CF3, OCF3, alkyl, alkoxy, etc.; R4 (optional) = H, halo, CN, CF3, OCF3, alkyl, alkoxy, etc.; X = C or N; R5 = H, alkyl, furyl, thienyl, styryl, pyridyl, (substituted)phenyl; R6 = H, alkyl,

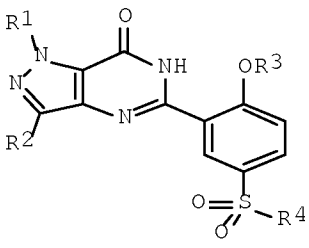
or -(CH2)n-X1-R7; n= 0-2; X1 = O, CO, CHOH, alkyl, or a single bond; R7 = an aromatic group optionally substituted with 1-3 substituents selected from H, halo, CN, CF3, OCF3, alkyl, alkoxy, etc.] were prepared as calcium receptor antagonists for the treatment of bone diseases. Thus, reaction of 2-phenyl-benzo[d][1,3]oxazin-4-one (preparation given) with phenethylamine gave compound II. Methods to determine the biol. activity of the compound of this invention were demonstrated.

IC ICM C07C
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

L79 ANSWER 10 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:565327 ZCAPLUS Full-text
DOCUMENT NUMBER: 146:521822
TITLE: Preparation of pyrazolopyrimidinone derivatives as inhibitors of type 5 phosphodiesterase
INVENTOR(S): Tian, Guanghui; Lai, Shunan; Wang, Zhen; Zhu, Yi; Chen, Xinjian; Ji, Yurong; Zhang, Jinfeng; Jin, Weixi; Lv, Heping; Liu, Jinping; Wang, Wei; Ji, Ruyun; Shen, Jingshan
PATENT ASSIGNEE(S): Topharman Shanghai Co., Ltd., Peop. Rep. China; Shanghai Institute of Materia Medica, Chinese Academy of Sciences; Henan Topfond Pharmaceutical Co., Ltd.
SOURCE: PCT Int. Appl., 66pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007056955	A1	20070524	WO 2006-CN3094	20061116
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW				
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
CN 1966506	A	20070523	CN 2005-10110485	20051117

PRIORITY APPLN. INFO.: CN 2005-10110485 A 20051117
OTHER SOURCE(S): MARPAT 146:521822
GI



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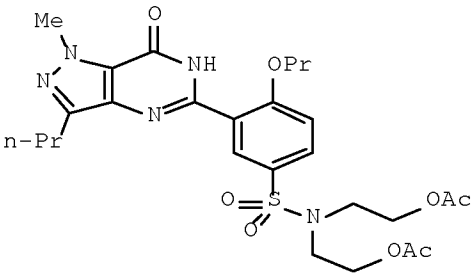

II

AB The title pyrazolopyrimidinone derivs. I [wherein R1 = H, (cyclo)alkyl, halogenated alkyl, or cycloalkyl substituted alkyl; R2 = (cyclo)alkyl, halogenated alkyl, or cycloalkyl substituted alkyl; R3 = (cyclo)alkyl, halogenated alkyl, alkoxyalkyl, or cycloalkyl substituted alkyl; R4 = substituted amino], or prodrugs, pharmaceutically acceptable salts, or solvates thereof were prepared as inhibitors of type 5 phosphodiesterase (PDE5). For example, 2-propoxy-5-[bis(2-acetoxyethyl)sulfamoyl]benzoic acid was reacted with 4-amino-1-methyl-3-propyl-1H-pyrazole-5-carboxamide, followed by cyclization to give II in high yield. II showed inhibitory activity with IC50 of 0.080 nM against PDE5. Formulations as capsules and tablets were described. The compds. are useful in improving or treating cardiovascular system or urinary system diseases (no data).

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

ST prepn pyrazolopyrimidinone phosphodiesterase inhibitor human

IT Angina pectoris
(Prinzmetal's; preparation of pyrazolopyrimidinone derivs. as PDE5 inhibitors)

IT Allergy
(allergic asthma; preparation of pyrazolopyrimidinone derivs. as PDE5 inhibitors)

IT Allergy
Inflammation
Nose, disease
(allergic rhinitis; preparation of pyrazolopyrimidinone derivs. as PDE5 inhibitors)

IT Asthma
(allergic; preparation of pyrazolopyrimidinone derivs. as PDE5 inhibitors)

IT Antiarteriosclerotics
(antiatherosclerotics; preparation of pyrazolopyrimidinone derivs. as PDE5 inhibitors)

IT Prostate gland, disease
(benign hyperplasia; preparation of pyrazolopyrimidinone derivs. as PDE5 inhibitors)

IT Hyperplasia
(benign prostatic; preparation of pyrazolopyrimidinone derivs. as PDE5 inhibitors)

IT Intestine, disease
(bowel movements; preparation of pyrazolopyrimidinone derivs. as PDE5 inhibitors)

IT Bronchi, disease
Inflammation
(bronchitis; preparation of pyrazolopyrimidinone derivs. as PDE5 inhibitors)

IT Asthma
(chronic; preparation of pyrazolopyrimidinone derivs. as PDE5 inhibitors)
IT Kidney, disease
(failure; preparation of pyrazolopyrimidinone derivs. as PDE5 inhibitors)
IT Sexual disorders
(female; preparation of pyrazolopyrimidinone derivs. as PDE5 inhibitors)
IT Sexual disorders
(impotence; preparation of pyrazolopyrimidinone derivs. as PDE5 inhibitors)
IT Bladder, disease
(incontinence; preparation of pyrazolopyrimidinone derivs. as PDE5 inhibitors)
IT Bladder, disease
(obstruction; preparation of pyrazolopyrimidinone derivs. as PDE5 inhibitors)
IT Blood vessel, disease
(peripheral; preparation of pyrazolopyrimidinone derivs. as PDE5 inhibitors)
IT Parturition disorders
(premature parturition; preparation of pyrazolopyrimidinone derivs. as PDE5 inhibitors)
IT Anti-inflammatory agents
Antiasthmatics
Antiglaucoma agents
Antihypertensives
Atherosclerosis
Cardiotonics
Dysmenorrhea
Gastrointestinal agents
Glaucoma
Heart failure
Human
Hypertension
Inflammation
Raynaud disease
Stroke
(preparation of pyrazolopyrimidinone derivs. as PDE5 inhibitors)
IT Hypertension
(pulmonary; preparation of pyrazolopyrimidinone derivs. as PDE5 inhibitors)
IT 936950-39-9P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of pyrazolopyrimidinone derivs. as PDE5 inhibitors)
IT 936950-40-2P 936950-41-3P 936950-42-4P 936950-43-5P 936950-44-6P
936950-45-7P 936950-46-8P 936950-47-9P 936950-48-0P 936950-49-1P
936950-50-4P 936950-51-5P 936950-52-6P 936950-53-7P 936950-54-8P
936950-55-9P 936950-56-0P 936950-57-1P 936950-58-2P 936950-59-3P
936950-60-6P 936950-61-7P 936950-62-8P 936950-63-9P 936950-64-0P
936950-65-1P 936950-66-2P 936950-67-3P 936950-68-4P 936950-69-5P
936950-70-8P 936950-71-9P 936950-72-0P 936950-73-1P 936950-74-2P
936950-75-3P 936950-76-4P 936950-77-5P 936950-78-6P 936950-79-7P
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936950-85-5P 936950-86-6P 936950-87-7P 936950-89-9P 936950-90-2P
936950-91-3P 936950-92-4P 936950-93-5P 936950-94-6P 936950-95-7P

936950-96-8P 936950-97-9P 936950-98-0P 936950-99-1P 936951-00-7P
936951-01-8P 936951-02-9P 936951-03-0P 936951-05-2P 936951-07-4P
936951-08-5P 936951-09-6P 936951-10-9P 936951-11-0P 936951-12-1P
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936951-18-7P 936951-19-8P 936951-20-1P 936951-21-2P 936951-22-3P
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936951-33-6P 936951-34-7P 936951-35-8P 936951-36-9P 936951-37-0P
936951-38-1P 936951-39-2P 936951-40-5P 936951-41-6P 936951-42-7P
936951-43-8P 936951-44-9P 936951-45-0P 936951-46-1P 936951-47-2P
936951-48-3P 936951-49-4P 936951-50-7P 936951-51-8P 936951-52-9P
936951-53-0P 936951-54-1P 936951-55-2P 936951-56-3P 936951-75-6P
936951-76-7P 936951-77-8P 936951-78-9P 936951-79-0P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of pyrazolopyrimidinone derivs. as PDE5 inhibitors)

IT 936951-57-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of pyrazolopyrimidinone derivs. as PDE5 inhibitors)

IT 139756-02-8 936951-58-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrazolopyrimidinone derivs. as PDE5 inhibitors)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 11 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2006:605352 ZCAPLUS Full-text
DOCUMENT NUMBER: 145:83371
TITLE: Preparation of prodrug constructs of pyrimidinone compounds as calcilytics
INVENTOR(S): Shcherbakova, Irina; Wermuth, Camille G.; Jeannot, Frederic; Ciapetti, Paola; Roques, Virginie; Jung, Laetitia M.; Balandrin, Manuel F.; Nair, Satheesh, K.; Swierczek, Krzysztof; McCaffrey, Jennifer; Heaton, William L.; Breinholt, Jeff A.; Conklin, Rebecca L.
PATENT ASSIGNEE(S): NPS Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 53 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006066070	A2	20060622	WO 2005-US45565	20051216
WO 2006066070	A3	20060921		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,

CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2004-637115P P 20041217

OTHER SOURCE(S): MARPAT 145:83371

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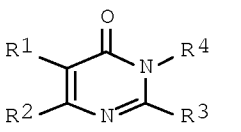

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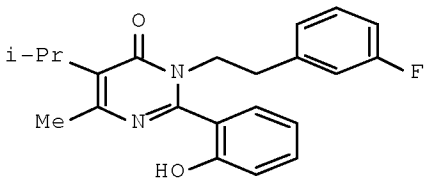


II

AB Calcilytic pyrimidinones I [R1 and R2 = H, halo, CN, CF3, etc.; R3 = (un)substituted aryl group; R4 = H, alkyl, aryl, etc.], and prodrugs as well as pharmaceutically acceptable salts thereof, are prepared for use in treating disease or disorders characterized by abnormal bone or mineral homeostasis. Thus, e.g., II was prepared by amidation of anisoyl chloride with 2-amino-2-isopropylbut-2-enoic acid Me ester (preparation given) followed by cyclization with 3-fluorphenethyl amine and demethylation. Calcilytic compds. are compds. capable of inhibiting calcium receptor activity. Assays for determining calcium receptor inhibition are described with parameter of desirable IC50 values given. Methods for preparing these compds., oral bioavailability of these compds., pharmaceutical compns. containing these compds. and their use as calcium receptor antagonists are also disclosed.

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

ST pyrimidinone deriv prepn calcilytic calcium receptor inhibitor; prodrug pyrimidinone deriv prepn calcilytic calcium receptor inhibitor

IT Bone, disease
(Paget's; preparation of prodrug constructs of pyrimidinone compound as calcilytics)

IT Receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(calcium, inhibition of; preparation of prodrug constructs of pyrimidinone compound as calcilytics)

IT Bone, disease
(fracture; preparation of prodrug constructs of pyrimidinone compound as calcilytics)

IT Mineral elements, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(homeostasis; preparation of prodrug constructs of pyrimidinone compound as calcilytics)

IT Neoplasm
(humoral hypercalcemia of malignancy; preparation of prodrug constructs of pyrimidinone compound as calcilytics)

IT Bone, neoplasm
Sarcoma
(osteosarcoma; preparation of prodrug constructs of pyrimidinone compound as calcilytics)

IT Antiosteoporotic agents
Antirheumatic agents
Antitumor agents

Bone, disease
Calcium channel blockers
Human
Osteoarthritis
Osteoporosis
Parathyroid gland, disease
Periodontium, disease
Pharmacokinetics
Rheumatoid arthritis
(preparation of prodrug constructs of pyrimidinone compound as calcilytics)

IT Drug delivery systems
(prodrugs; preparation of prodrug constructs of pyrimidinone compound as calcilytics)

IT 9002-64-6, Parathyroid hormone
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(increasing serum parathyroid hormone levels; preparation of prodrug constructs of pyrimidinone compound as calcilytics)

IT 780771-48-4P 893053-18-4P 893053-34-4P 893054-04-1P 893054-20-1P
893054-36-9P 893054-44-9P 893054-51-8P 893054-67-6P
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of prodrug constructs of pyrimidinone compound as calcilytics)

IT 893053-26-4P 893053-42-4P 893053-50-4P 893053-57-1P 893053-65-1P
893053-73-1P 893053-81-1P 893053-88-8P 893053-96-8P 893054-12-1P
893054-28-9P 893054-59-6P 893054-75-6P
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of prodrug constructs of pyrimidinone compound as calcilytics)

IT 893054-83-6P 893054-91-6P 893054-99-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of prodrug constructs of pyrimidinone compound as calcilytics)

IT 78-84-2, Isobutyryl aldehyde 79-30-1, Isobutyryl chloride 105-45-3, Methyl acetoacetate 108-23-6, Isopropyl chloroformate 404-70-6, 3-Fluorophenethyl amine 541-41-3, Ethyl chloroformate 595-37-9, 2,2-Dimethylbutyric acid 610-14-0, 2-Nitrobenzoyl chloride 1522-34-5 1522-46-9, 2-Acetyl-3-methylbutyric acid ethyl ester 1655-07-8, Ethyl 2-oxocyclohexanecarboxylate 1730-91-2, (S)-2-Methylbutyric acid 3282-30-2, Pivaloyl chloride 7065-46-5, tert-Butylacetyl chloride 17176-77-1, Dibenzylphosphite 21615-34-9, 2-Anisoyl chloride 24424-99-5, Di-tert-butyl dicarbonate 106428-06-2, 3-Fluoro-2-methoxybenzoyl chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of prodrug constructs of pyrimidinone compound as calcilytics)

IT 51756-10-6P 57205-09-1P 58019-68-4P 86577-04-0P 780771-51-9P
893055-14-6P 893055-22-6P 893055-45-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of prodrug constructs of pyrimidinone compound as calcilytics)

L79 ANSWER 12 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2005:1106804 ZCAPLUS Full-text
DOCUMENT NUMBER: 143:387057
TITLE: Preparation of pyrimidinone derivatives as mitotic kinesin inhibitors
INVENTOR(S): Wang, Weibo; Constantine, Ryan; Lagniton, Liana
PATENT ASSIGNEE(S): Chiron Corporation, USA
SOURCE: U.S. Pat. Appl. Publ., 32 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 20050228002	A1	20051013	US 2005-100923		20050406
AU 2005233576	A1	20051027	AU 2005-233576		20050406
CA 2561904	A1	20051027	CA 2005-2561904		20050406
WO 2005100357	A1	20051027	WO 2005-US11642		20050406
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
EP 1732926	A1	20061220	EP 2005-732607		20050406
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, AL, BA, HR, LV, MK, YU					
CN 1984912	A	20070620	CN 2005-80017432		20050406
BR 2005009653	A	20071009	BR 2005-9653		20050406
JP 2007532554	T	20071115	JP 2007-507466		20050406
MX 2006PA11464	A	20061207	MX 2006-PA11464		20061004
IN 2006KN02877	A	20070608	IN 2006-KN2877		20061005
PRIORITY APPLN. INFO.:			US 2004-560235P	P	20040406
			WO 2005-US11642	W	20050406

OTHER SOURCE(S): CASREACT 143:387057; MARPAT 143:387057
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [R1 = halo, aryl, CN, etc.; R2 = H, alkyl, alkenyl, etc.; R3 = alkyl, alkynyl, heterocycle, etc.; R2 and R3 together may form carbocyclic or heterocyclic ring wherein 1-3 ring atoms are selected from N, O and S; R4 = H, alkyl, aryl, etc.; R5 = alkoxycarbonyl, aminocarbonyl, alkylsulfonyl, etc.; R6 = H, OH, NH2, etc.; R7 = H, alkyl, heterocycle, etc.; R6 and R7 together may form heterocyclic ring containing 1-3 ring atoms selected from N, O and S] and their pharmaceutically acceptable salts, are prepared and disclosed as inhibitors of mitotic kinesin. Thus, e.g., II was prepared by alkylation of 2-(1-amino-2-methylpropyl)-3-benzyl-6,7,8,9- tetrahydro-4H-pyrido[1,2-

a]pyrimidin-4-one (preparation given) with phthalimide protected 3-aminopropionaldehyde followed by benzoylation using 4-Me benzoyl chloride and subsequent deprotection. The inhibitory activity of I was evaluated using spectrophotometric assay using the motor domain of human KSP (no data). I should prove useful in the treatment of cancers such as but not limited to breast, prostate and lung. Pharmaceutical compns. comprising I are disclosed.

IC ICM A61K031-519
ICS C07D489-02
INCL 514259400; 544281000; 514259410
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63
ST pyrimidinone prepn inhibitor mitotic kinesin antitumor
IT Lymphoma
(B-cell; preparation of pyrimidinone derivs. as mitotic kinesin inhibitors)
IT Esophagus, neoplasm
Uterus, neoplasm
(adenocarcinoma; preparation of pyrimidinone derivs. as mitotic kinesin inhibitors)
IT Uterus, neoplasm
(cervix; preparation of pyrimidinone derivs. as mitotic kinesin inhibitors)
IT Intestine, neoplasm
(colon, adenoma; preparation of pyrimidinone derivs. as mitotic kinesin inhibitors)
IT Intestine, neoplasm
(colon; preparation of pyrimidinone derivs. as mitotic kinesin inhibitors)
IT Adenoma
(colonic; preparation of pyrimidinone derivs. as mitotic kinesin inhibitors)
IT Carcinoma
(esophageal adenocarcinoma; preparation of pyrimidinone derivs. as mitotic kinesin inhibitors)
IT Pharynx, neoplasm
(nasopharynx; preparation of pyrimidinone derivs. as mitotic kinesin inhibitors)
IT Kidney
(pelvis, neoplasm; preparation of pyrimidinone derivs. as mitotic kinesin inhibitors)
IT Antitumor agents
Bile duct, neoplasm
Bladder, neoplasm
Brain, neoplasm
Chronic myeloid leukemia
Human
Kidney, neoplasm
Larynx, neoplasm
Liver, neoplasm
Lung, neoplasm
Lymphocytic leukemia
Mammary gland, neoplasm
Melanoma
Mouth, neoplasm
Multiple myeloma
Myeloid leukemia
Neoplasm
Ovary, neoplasm
Pancreas, neoplasm
Prostate gland, neoplasm

Stomach, neoplasm
Thyroid gland, neoplasm
(preparation of pyrimidinone derivs. as mitotic kinesin inhibitors)

IT Kinesins
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(preparation of pyrimidinone derivs. as mitotic kinesin inhibitors)

IT Intestine, neoplasm
(rectum; preparation of pyrimidinone derivs. as mitotic kinesin inhibitors)

IT Intestine, neoplasm
(small; preparation of pyrimidinone derivs. as mitotic kinesin inhibitors)

IT Carcinoma
(uterine adenocarcinoma; preparation of pyrimidinone derivs. as mitotic kinesin inhibitors)

IT 50-18-0, Cyclophosphamide 51-21-8, 5-Fluorouracil 58-05-9, Leucovorin 15663-27-1, Cisplatin 33069-62-4, Paclitaxel 41575-94-4, Carboplatin 95058-81-4, Gemcitabine 97682-44-5, Irinotecan 114977-28-5, Docetaxel 123948-87-8, Topotecan 130306-02-4, Tezacitabine 152459-95-5, Imatinib 174722-31-7, Rituximab 180288-69-1, Trastuzumab
RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(claimed co-drug; preparation of pyrimidinone derivs. as mitotic kinesin inhibitors)

IT 866611-03-2P 866611-05-4P 866611-07-6P 866611-09-8P 866611-11-2P 866611-13-4P 866611-14-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidinone derivs. as mitotic kinesin inhibitors)

IT 85-41-6, Phthalimide 504-29-0, 2-Aminopyridine 586-75-4, 4-Bromobenzoyl chloride 638-07-3, Ethyl 4-Chloroacetoacetate 874-60-2, 4-Methyl benzoyl chloride 1826-67-1, Vinyl magnesium bromide 2436-29-5 13291-18-4, Isopropenylmagnesium bromide 53317-09-2, B-Benzyl-9-BBN 59189-97-8 75178-96-0, tert-Butyl-3-aminopropylcarbamate 866611-26-9 1037587-20-4
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrimidinone derivs. as mitotic kinesin inhibitors)

IT 16867-35-9P 817204-59-4P 817205-98-4P 817205-99-5P 817206-00-1P 817206-01-2P 817206-02-3P 866611-15-6P 866611-16-7P 866611-17-8P 866611-18-9P 866611-19-0P 866611-20-3P 866611-21-4P 866611-22-5P 866611-23-6P 866611-24-7P 866611-25-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrimidinone derivs. as mitotic kinesin inhibitors)

L79 ANSWER 13 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:1154708 ZCAPLUS Full-text
DOCUMENT NUMBER: 142:93843
TITLE: Preparation of pyrido[1,2-a]pyrimidin-4-ones as anticancer agents
INVENTOR(S): Wang, Weibo; Constantine, Ryan N.; Lagniton, Liana M.; Pecchi, Sabina; Burger, Matthew T.; Desai, Manoj C.
PATENT ASSIGNEE(S): Chiron Corporation, USA
SOURCE: PCT Int. Appl., 78 pp.

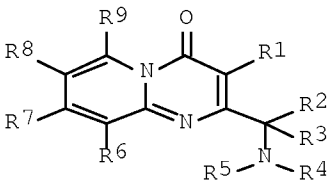
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004113335	A2	20041229	WO 2004-US19158	20040617
WO 2004113335	A3	20050324		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004249730	A1	20041229	AU 2004-249730	20040617
CA 2528771	A1	20041229	CA 2004-2528771	20040617
US 20050085490	A1	20050421	US 2004-870707	20040617
US 7326711	B2	20080205		
EP 1636225	A2	20060322	EP 2004-776639	20040617
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
CN 1809563	A	20060726	CN 2004-80017139	20040617
JP 2007520435	T	20070726	JP 2006-517308	20040617
IN 2005KN02472	A	20061013	IN 2005-KN2472	20051202
MX 2005PA13142	A	20060317	MX 2005-PA13142	20051205

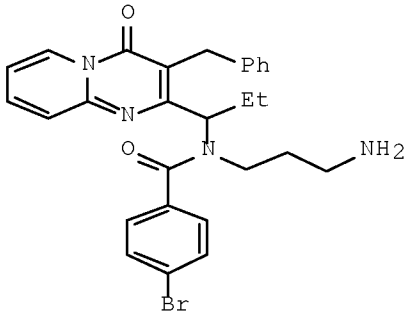
PRIORITY APPLN. INFO.: US 2003-480180P P 20030620
WO 2004-US19158 W 20040617

OTHER SOURCE(S): MARPAT 142:93843

GI



I



II

AB The title compds. I [R1 = H, alkyl, aryl, etc.; R2, R3 = H, alkyl, aryl, etc.; or R2 and R3 taken together with the carbon atom to which they are attached form a 3-7 membered carbocyclic or heterocyclic ring; R4 = H, alkyl, aryl, etc.; R5 = H, alkyl, aryl, etc.; R6-R9 = H, halo, NO2, etc.], useful, either

alone or in combination with at least one addnl. therapeutic agent, in the prophylaxis or treatment of proliferative diseases, were prepared E.g., a multi-step synthesis of II, starting from 2-aminopyridine and Et 4-chloroacetoacetate, was given. Certain compds. I were shown to have a KSP inhibitory activity at an IC50 of less than about 25 μM. The compns. that include a pharmaceutically acceptable carrier and one or more of the pyrido[1,2-a]pyrimidinyl compds. I, either alone or in combination with at least one addnl. therapeutic agent, were disclosed.

IC ICM C07D471-00
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63
ST pyridopyrimidinone prepn antitumor KSP kinesis inhibitor

L79 ANSWER 14 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:1127387 ZCAPLUS Full-text
DOCUMENT NUMBER: 142:74600
TITLE: Heteroaryl-fused pyrimidinyl compounds, including thieno[3,2-d]pyrimidine derivatives, with KSP-inhibiting activity, and their preparation, pharmaceutical compositions, and use as anticancer agents
INVENTOR(S): Wang, Weibo; Lagniton, Liana M.; Constantine, Ryan N.; Burger, Matthew T.
PATENT ASSIGNEE(S): Chiron Corporation, USA
SOURCE: PCT Int. Appl., 59 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004111058	A1	20041223	WO 2004-US16954	20040527
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 20050065169	A1	20050324	US 2004-850429	20040521
US 7345046	B2	20080318		
AU 2004247650	A1	20041223	AU 2004-247650	20040527
CA 2526217	A1	20041223	CA 2004-2526217	20040527
EP 1636238	A1	20060322	EP 2004-753729	20040527
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
CN 1798749	A	20060705	CN 2004-80014819	20040527
JP 2007500237	T	20070111	JP 2006-533499	20040527
IN 2005KN02291	A	20070316	IN 2005-KN2291	20051117
MX 2005PA12706	A	20060208	MX 2005-PA12706	20051124
US 20080069817	A1	20080320	US 2007-863048	20070927

PRIORITY APPLN. INFO.:	US 2003-474684P	P	20030530
	US 2004-850429	A3	20040521
	WO 2004-US16954	W	20040527

OTHER SOURCE(S): MARPAT 142:74600
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Heteroaryl-fused pyrimidinyl compds. and their pharmaceutically acceptable salts and prodrugs are disclosed. The compds. are KSP inhibitors, useful in the treatment of cellular proliferative diseases. Also disclosed are compns. that include a pharmaceutically acceptable carrier and one or more invention compds., either alone or in combination with at least one addnl. therapeutic agent. Methods of using the invention compds., either alone or in combination with at least one addnl. therapeutic agent, in the prophylaxis or treatment of proliferative diseases, are also disclosed. The disclosed compds. are covered by I [wherein Q = heteroaryl fusion; X = O or S; R1 = H, (un)substituted alk(en/yn)yl, (hetero)aryl, heterocyclyl, (alkyl/aryl)sulfonyl; R2 = H, (un)substituted alk(en/yn)yl, (hetero)aryl, heterocyclyl, (alkyl/aryl)sulfonyl, alkylcarboxy, aminocarboxy, aminocarbonyl, alkylsulfonamido, COR7, CO2R7, CONR8R9, S(O)mR10, or SO2NR11R12; R3 = cyano, (un)substituted arylsulfonyl, or CONR8R9; R4 = H, (un)substituted alk(en/yn)yl, (hetero)aryl, heterocyclyl, L-R13; L = C1-10 (un)saturated (un)branched C chain comprising 1 or more methylene groups, wherein 1 or more methylene groups is optionally replaced by O, N, or S, and wherein L is optionally substituted with 1 or 2 oxos and 1 or more C1-10 branched or unbranched alkyl (un)substituted by 1 or more halo atoms; R5 = H, (un)substituted alk(en/yn)yl, alkoxy, (hetero)aryl, or heterocyclyl, COR7, CO2R7, CONR8R9, or SOmR10; R6 = H, halo, OH, NO2, amino, cyano, (halo)alkoxy, alkylthio, methylenedioxy, (un)substituted alk(en/yn)yl, (hetero)aryl, (di)alkylamino, (alkyl/aryl)sulfonyl, alkylcarboxy, carboxyamino, carboxyamido, aminocarboxy, aminocarbonyl, or alkylsulfonamido; R7, R8, R9, R10, R11, R12 = H, or (un)substituted alk(en/yn)yl, (hetero)aryl, or heterocyclyl; or R89 or R11R12 = 3- to 7-membered (carbo/hetero)cyclic ring; R13 = (di)(alkyl)amino, (un)substituted guanidino or heterocyclyl; m = 0-2; and n = 0-3; or tautomers, pharmaceutically acceptable salts, or prodrugs]. Six example compds., one salt, and six intermediates are described. For example, Me 3-amino-2-thiophenecarboxylate was brominated in the 5-position (57%), and the resulting amino ester was cyclocondensed with 2-cyano-N,N-dimethylacetamide to give thieno[3,2-d]pyrimidinone intermediate II. This compound underwent N-benzylation (39%), followed by α-bromination of the amide (90%), amination of the bromide with Boc-NH(CH2)3NH2 (34%), amidation of the obtained amine with 4-MeC6H4COCl (64%), and removal of Boc with HCl (52%), to give title compound III. In an assay for KSP activity using the cloned motor domain of human KSP, the six compds. I showed Eg5 inhibitory activity with IC50 of < 25 μM, with some compds. said to show IC50 of less than 1 μM.

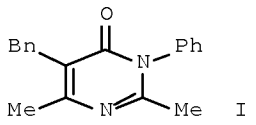
IC ICM C07D495-04
ICS A61K031-519; A61P035-00

CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 15 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:147199 ZCAPLUS Full-text
DOCUMENT NUMBER: 140:339284
TITLE: An efficient synthesis of 3-substituted 3H-pyrimidin-4-ones
AUTHOR(S): Jeong, Jae Uk; Chen, Xiaohong; Rahman, Attiq; Yamashita, Dennis S.; Luengo, Juan I.

CORPORATE SOURCE: Department of Medicinal Chemistry, MMPD CEDD, GlaxoSmithKline, Collegeville, PA, 19426, USA
SOURCE: Organic Letters (2004), 6(6), 1013-1016
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:339284
GI



I

AB A practical synthesis of 3-substituted 3H-pyrimidin-4-ones, e.g., I, is described. The key step involved the cyclization of enamide esters, derived from readily available β-keto esters, with various primary amines.
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
ST enamide ester amine heterocyclization; pyrimidinone prepn
IT Carboxylic acids, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxo, esters; preparation of pyrimidinones via condensation of ammonium acetate with β-keto esters followed by amidation with anhydrides and heterocyclization with primary amines)
IT Heterocyclization
(preparation of pyrimidinones via condensation of ammonium acetate with β-keto esters followed by amidation with anhydrides and heterocyclization with primary amines)
IT Amines, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(primary; preparation of pyrimidinones via condensation of ammonium acetate with β-keto esters followed by amidation with anhydrides and heterocyclization with primary amines)
IT 680860-31-5P
RL: BYP (Byproduct); PREP (Preparation)
(byproduct from the preparation of pyrimidinones via condensation of ammonium acetate with β-keto esters followed by acylation with anhydrides and heterocyclization with amines)
IT 680860-29-1P 680860-30-4P
RL: BYP (Byproduct); PREP (Preparation)
(byproducts from the preparation of benzyl(dimethyl)oxazinone via heterocyclization of acetamido(benzyl)butenoate in the attempted preparation
of pyrimidinones)
IT 136744-85-9P
RL: BYP (Byproduct); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-(benzyl)dimethylpyrimidinone via heterocyclization of acetamidobutenoate with benzylamine)
IT 680860-28-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of benzyl(dimethyl)oxazinone via heterocyclization of acetamido(benzyl)butenoate in the attempted preparation of

pyrimidinones)
IT 117838-64-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of benzyl(diphenyl)methylpyrimidinone via heterocyclization of benzoylamido(benzyl)butenoate followed by rearrangement with aniline)
IT 62-53-3, Aniline, reactions 93-97-0, Benzoic anhydride 100-46-9, Benzylamine, reactions 105-45-3, Methyl 3-oxobutanoate 108-91-8, Cyclohexylamine, reactions 609-14-3, Ethyl 2-methyl-3-oxobutanoate 620-79-1, Ethyl 2-benzyl-3-oxobutanoate 6291-85-6, 3-Ethoxypropylamine
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of pyrimidinones via condensation of ammonium acetate with β-keto esters followed by amidation with anhydrides and heterocyclization with primary amines)
IT 67654-56-2P 680860-17-7P 680860-18-8P 680860-19-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of pyrimidinones via condensation of ammonium acetate with β-keto esters followed by amidation with anhydrides and heterocyclization with primary amines)
IT 32363-53-4P 69912-32-9P 680860-20-2P 680860-21-3P 680860-22-4P 680860-23-5P 680860-24-6P 680860-25-7P 680860-26-8P 680860-27-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of pyrimidinones via condensation of ammonium acetate with β-keto esters followed by amidation with anhydrides and heterocyclization with primary amines)
REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L79 ANSWER 16 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:227011 ZCAPLUS Full-text
TITLE: Efficient synthesis of 3-substituted pyrimidinones
AUTHOR(S): Jeong, Jae Uk; Chen, Xiaohong; Rahman, Attiq; Yamashita, Dennis S.; Luengo, Juan I.
CORPORATE SOURCE: Medicinal Chemistry, GlaxoSmithKline Pharm, Collegeville, PA, 19426, USA
SOURCE: Abstracts of Papers, 227th ACS National Meeting, Anaheim, CA, United States, March 28-April 1, 2004 (2004), ORGN-140. American Chemical Society: Washington, D. C.
CODEN: 69FGKM
DOCUMENT TYPE: Conference; Meeting Abstract
LANGUAGE: English
AB Many biol. active compds. such as PPAR agonists and angiotensin antagonists contain 3-substituted pyrimidinones. A novel and efficient synthesis of 3-substituted pyrimidinones has been developed. The key step involves the cyclization of enamides, derived from readily available beta-keto esters, with trimethylaluminum and various primary amines. The general procedure, scope and application of this synthetic method will be discussed.

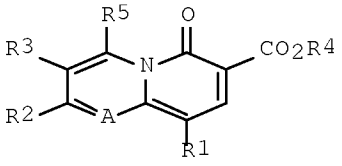
L79 ANSWER 17 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1997:116497 ZCAPLUS Full-text
DOCUMENT NUMBER: 126:117990
ORIGINAL REFERENCE NO.: 126:22777a,22780a
TITLE: Preparation of quinolizinone- and pyridopyrimidinonecarboxylates as antibacterials
INVENTOR(S): Chu, Daniel T.; Li, Qun; Cooper, Curt S.; Fung,

Anthony K. L.; Lee, Cheuk M.; Plattner, Jacob J.; Ma, Zhenkun; Wang, Wei-Bo
PATENT ASSIGNEE(S): Abbott Laboratories, USA
SOURCE: PCT Int. Appl., 412 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9639407	A1	19961212	WO 1996-US8991	19960605
W: AU, CA, IL, JP, KP, MX				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2222322	A1	19961212	CA 1996-2222322	19960605
AU 9661530	A	19961224	AU 1996-61530	19960605
EP 871628	A1	19981021	EP 1996-919103	19960605
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI				
JP 11510478	T	19990914	JP 1996-501420	19960605

PRIORITY APPLN. INFO.: US 1995-469159 A 19950606
US 1996-638112 A 19960529
WO 1996-US8991 W 19960605

OTHER SOURCE(S): MARPAT 126:117990
GI



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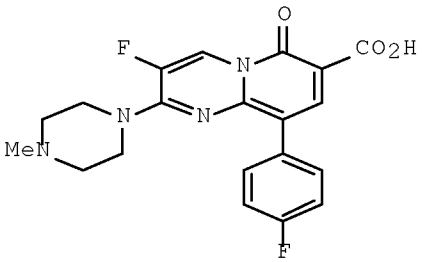

II

AB Title compds. [I; A = N or CR6; R1 = halo, (cyclo)alkyl, alkoxy, (un)substituted Ph, etc.; R2 = halo, (cyclo)alkyl, alkoxy, N-containing heterocyclyl, etc.; R3 = H, halo, alkoxy; R4 = H, alkyl, cation, etc.; R5,R6 = H, halo, alkyl, alkoxy, etc.] were prepared Thus, 4-FC6H4CH2C(:NH)NH2 was cyclocondensed with NaOCH:CFCO2Et (preparation given) and the chlorinated product aminated by 1-methylpiperazine to give 5-fluoro-2-(4-fluorobenzyl)-4-(4-methylpiperazino)pyrimidine which was condensed with EtOCH:C(CO2Et)2 and the product cyclized to give, in 2 addnl. steps, title compound II. Data for biol. activity of I were given.
IC ICM C07D471-04
ICS C07D455-02; C07D491-16; C07D519-00; A61K031-435; A61K031-505; C07D213-68; C07D213-61
ICI C07D471-04, C07D239-00, C07D221-00; C07D519-00, C07D487-00, C07D455-00; C07D519-00, C07D491-00, C07D471-00; C07D491-16, C07D311-00, C07D221-00
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

ST pyridopyrimidinonecarboxylate quinolizinonecarboxylate prepn antibacterial

IT Antibacterial agents
(quinolizinone- and pyridopyrimidinonecarboxylates)

IT 139160-76-2P 139160-77-3P 139160-80-8P 139160-81-9P 139160-82-0P
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RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of quinolizinone- and pyridopyrimidinonecarboxylates as antibacterials)

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186293-38-9P 186293-39-0P 186293-50-5P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of quinolizinone- and pyridopyrimidinonecarboxylates as antibacterials)

IT 18368-63-3P, 6-Chloro-2-picoline
RL: BYP (Byproduct); PREP (Preparation)
(preparation of quinolizinone- and pyridopyrimidinonecarboxylates as antibacterials)

IT 78-89-7, 2-Chloro-1-propanol 85-41-6, Phthalimide 87-13-8, Diethyl ethoxymethylenemalonate 87-52-5 91-21-4 96-33-3, Methyl acrylate 100-46-9, Benzylamine, reactions 100-51-6, Benzyl alcohol, reactions 104-63-2 105-53-3, Diethyl malonate 106-89-8, reactions 107-12-0, Propionitrile 109-01-3, 1-Methylpiperazine 109-07-9, 2-Methylpiperazine 109-97-7, Pyrrole 110-91-8, Morpholine, reactions 123-38-6, Propionaldehyde, reactions 140-29-4, Benzeneacetonitrile 288-32-4, Imidazole, reactions 381-98-6, 2-(Trifluoromethyl)acrylic acid 459-72-3 494-52-0, Anabasine 501-53-1, Benzyl chloroformate 505-66-8, Homopiperazine 524-38-9, N-Hydroxyphthalimide 653-30-5, Pentafluorophenylacetonitrile 656-35-9, 2,4-Difluorophenylacetonitrile 696-59-3 699-98-9, Furo[3,4-b]pyridine-5,7-dione 700-16-3, Pentafluoropyridine 765-30-0, Cyclopropylamine 765-43-5, Cyclopropyl methyl ketone 775-16-6, 1-Benzyl-3-pyrrolidinone 865-48-5, Sodium tert-butoxide 931-19-1 1099-45-2 1122-58-3, 4-(Dimethylamino)pyridine 1125-60-6, 5-Isoquinolinamine 1191-95-3, Cyclobutanone 1522-41-4, Ethyl 2-fluoro-3-oxobutanoate 1631-26-1, N-Benzylmaleimide 1735-84-8, 3-Chloro-2,4,5,6-tetrafluoropyridine 2049-67-4, Diethyl glutaconate 2562-37-0, 1-Nitrocyclohexene 2766-43-0 3401-36-3 3612-20-2 3731-52-0, 3-Pyridinemethanamine 4548-45-2, 2-Chloro-5-nitropyridine 4606-65-9, 3-(Hydroxymethyl)piperidine 4704-77-2, 3-Bromo-1,2-propanediol 4727-72-4 4897-50-1, 1,4'-Bipiperidine 5192-03-0, 5-Aminoindole 5291-77-0, 1-Benzyl-2-pyrrolidinone 5382-16-1, 4-Piperidinol 5470-18-8 5808-99-1, Ethyl 3-cyclopropylacrylate 6600-40-4, Norvaline 6859-99-0, 3-Hydroxypiperidine 7144-05-0, 4-Piperidinemethanamine 10029-04-6 15014-25-2, Dibenzyl malonate 15336-72-8, 4,4'-Bipiperidine 16012-70-7, N-Benzyloxycarbonyl-alanylalanine 18471-40-4 21655-48-1 23356-96-9 25597-16-4 31970-04-4 32864-38-3, Ethyl tert-butyl malonate 33403-97-3 34803-66-2 36476-88-7, 3-Aminomethyl-1-diphenylmethylazetidine 40114-49-6 40499-83-0, 3-Pyrrolidinol 42392-67-6 50882-16-1, 2-Oxocyclopentanecarboxylic acid 51594-55-9,

(R)-Epichlorohydrin, reactions 51628-01-4, 4-Fluorophenylacetamidine hydrochloride 62414-68-0 64051-79-2, 3-Hydroxypiperidine hydrochloride 68832-13-3 69478-75-7 71447-85-3 72657-23-9, (R)-Methyl 3-hydroxy-2-methylpropionate 75272-49-0 89031-84-5, 3-Bromo-1-(tert-butyldimethylsilyloxy)propane 91188-13-5 98244-48-5, (S)-3-Bromo-2-methyl-1-propanol 99724-19-3, 3-(tert-Butoxycarbonylamino)pyrrolidine 101385-90-4 104587-62-4 107610-64-0, cis-3-(tert-Butoxycarbonylamino)-4-methylpyrrolidine 107610-69-5 113451-55-1 113451-59-5 122536-76-9 123844-20-2, Ethyl 3-cyclopropylpropiolate 128740-18-1 130658-47-8 132414-81-4 132958-72-6 139161-94-7, 4-Chloro-3,5-difluoro-2-methylpyridine 143444-83-1 143700-03-2 147459-52-7 150395-91-8 155497-06-6 169750-89-4 169750-92-9 185693-07-6 185693-09-8 186203-81-6 186203-82-7 186203-91-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of quinolizinone- and pyridopyrimidinonecarboxylates as antibacterials)

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169750-54-3P 169750-55-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of quinolizinone- and pyridopyrimidinonecarboxylates as antibacterials)

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186202-46-0P 186202-49-3P 186202-51-7P 186202-54-0P 186202-57-3P
186202-59-5P 186202-66-4P 186202-68-6P 186202-73-3P 186202-79-9P
186202-81-3P 186202-83-5P 186202-85-7P 186202-87-9P 186202-89-1P
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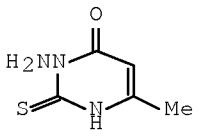
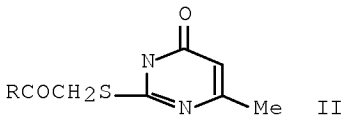
186203-26-9P 186203-28-1P 186203-30-5P 186203-32-7P 186203-34-9P
186203-36-1P 186203-37-2P 186203-38-3P 186203-41-8P 186203-43-0P
186203-46-3P 186203-47-4P 186203-49-6P 186203-51-0P 186203-53-2P
186203-55-4P 186203-58-7P 186203-60-1P 186203-62-3P 186203-63-4P
186203-64-5P 186203-66-7P 186203-67-8P 186203-68-9P 186203-69-0P
186203-70-3P 186203-71-4P 186203-72-5P 186203-73-6P 186203-74-7P
186203-75-8P 186203-76-9P 186203-77-0P 186203-78-1P 186203-79-2P
186203-80-5P 186203-92-9P 186293-54-9P 186293-55-0P 186293-56-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of quinolizinone- and pyridopyrimidinonecarboxylates as antibacterials)

L79 ANSWER 18 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1992:571362 ZCAPLUS Full-text
DOCUMENT NUMBER: 117:171362
ORIGINAL REFERENCE NO.: 117:29629a,29632a
TITLE: Antiviral activity of pyrimidinyl-2-thioacetic acid derivatives
AUTHOR(S): Koksharova, T. G.; Volkova, N. V.; Dianova, L. N.; Il'enko, V. I.; Platonov, V. G.; Shcherbakova, I. R.
CORPORATE SOURCE: Ural. Politekh. Inst., Yekaterinburg, Russia
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1992), 26(3), 57-9

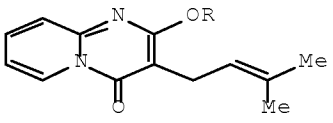
CODEN: KHFZAN; ISSN: 0023-1134
DOCUMENT TYPE: Journal
LANGUAGE: Russian
GI

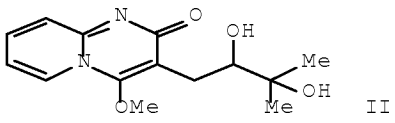

I


II

AB Reaction of thioxopyrimidinone I with BrCH2CO2H gave title compound II (R = HO), which was also obtained by reaction of I with ClCH2CO2R1 (R1 = Me, Et), followed by saponification Reaction of II (R = HO) with aldehydes gave imine-containing carboxylic acids, and reaction of II (R = MeO, EtO) with N2H4 gave II (R = H2NNH), which formed hydrazones with aldehydes. Of the compds. tested, II (R = H2NNH) had the highest antiviral activity.
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
IT 79-08-3, Bromoacetic acid 96-34-4, Methyl chloroacetate 105-39-5, Ethyl chloroacetate
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with aminothioxopyrimidinone)

L79 ANSWER 19 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1990:98480 ZCAPLUS Full-text
DOCUMENT NUMBER: 112:98480
ORIGINAL REFERENCE NO.: 112:16751a,16754a
TITLE: Synthesis of pyrido[1,2-a]pyrimidinone series of compounds, potential agents on the nervous system
AUTHOR(S): Wang, W. G.; Qian, L. G.; Ji, R. Y.
CORPORATE SOURCE: Shanghai Inst. Mater. Med., Acad. Sin., Shanghai, 200031, Peop. Rep. China
SOURCE: Yaoxue Xuebao (1989), 24(5), 393-6
CODEN: YHHPAL; ISSN: 0513-4870
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
GI

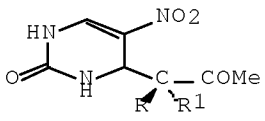

I


II

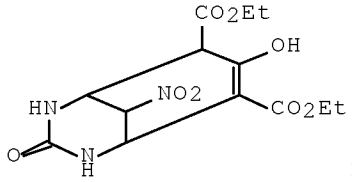
AB Title compds., e.g., I (R = H, Me) and II, were prepared starting from 2-aminopyridine and di-Et 3-methyl-2-butenylmalonate. Compd I (R = Me) showed anticonvulsant activity.
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

ST aminopyridine cyclocondensation methylbutenylmalonate; pyridopyrimidinone prepn anticonvulsant
IT Anticonvulsants and Antiepileptics
(pyridopyrimidinone derivs.)

L79 ANSWER 20 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1982:104170 ZCAPLUS Full-text
DOCUMENT NUMBER: 96:104170
ORIGINAL REFERENCE NO.: 96:17109a,17112a
TITLE: Pyrimidines. 18. A novel pyrimidine to benzene ring transformation reaction. Conversion of 5-nitro-2(1H)-pyrimidinone into p-nitrophenol derivatives
AUTHOR(S): Fox, Jack J.; Su, Tsann Long; Stempel, Lloyd M.; Watanabe, Kyoichi
CORPORATE SOURCE: Sloan-Kettering Inst. Cancer Res., Cornell Univ., New York, NY, 10021, USA
SOURCE: Journal of Organic Chemistry (1982), 47(6), 1081-4
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 96:104170
GI



II, R=Me, R1=H
III, R1=H, R=Me

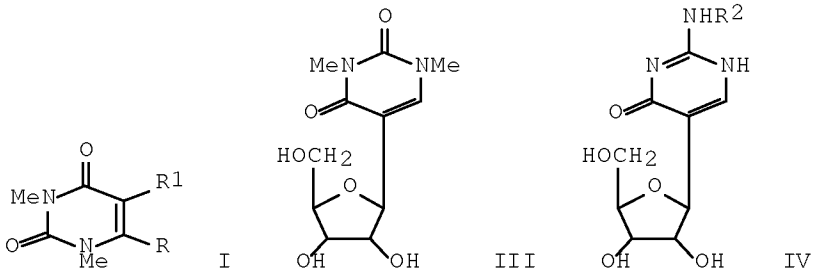


IV

AB 5-Nitro-2(1H)-pyrimidinone (I) underwent acid-catalyzed condensation with acetone and Et acetoacetate to form 4-ketonyl-5-nitropyrimidines, which were readily converted into p-nitrophenol and 5-nitrosalicylic acid, resp., by NaOH treatment. Condensation of I with butanone gave a pair of diastereomeric adducts II and III, which upon base treatment afforded 4-nitrocresol. Acid-catalyzed reaction of I with di-Et acetonedicarboxylate gave IV, which underwent base-catalyzed conversion into 2-hydroxy-5-nitroisophthalic acid. Treatment of 1-methyl-4-nitro- 2(1H)-pyrimidinone with acetone in the presence of acid afforded 4-acetonyl-3-methyl and 4-acetonyl-1-methyl adducts, which were converted sep. into III. Identification and characterization of the ketonyl adducts are reported. Reaction mechanisms are proposed.
CC 28-16 (Heterocyclic Compounds (More Than One Hetero Atom))
ST pyrimidinone nitro ring transformation; ring transformation nitropyrimidinone; phenol nitro; nitrophenol; diazabicyclononenedicarboxylate ring cleavage
IT 96-97-9P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, by ring transformation of pyrimidinone derivative)

L79 ANSWER 21 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1978:121634 ZCAPLUS Full-text

DOCUMENT NUMBER: 88:121634
ORIGINAL REFERENCE NO.: 88:19109a,19112a
TITLE: Pyrimidines. 14. Novel pyrimidine to pyrimidine transformation reactions and their application to C-nucleoside conversions. A facile synthesis of pseudoisocytidine
AUTHOR(S): Hirota, Kosaku; Watanabe, Kyoichi A.; Fox, Jack J.
CORPORATE SOURCE: Grad. Sch. Med. Sci., Cornell Univ., New York, NY, USA
SOURCE: Journal of Organic Chemistry (1978), 43(6), 1193-7
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Novel pyrimidine to pyrimidine transformations by nucleophilic displacement of the N-1-C-2-N-3 portion of 1,3-dialkyluracils [I; R = H, R1 = H (II), Me, F; R = Me, R1 = H, Br] by the N-C-N fragment of several 1,3-ambident nucleophiles were investigated. Treatment of II with guanidine in refluxing EtOH afforded 2-amino-4(3H)-pyrimidinone. The ease with which the reaction occurs depends on the electronic nature of the substituent at C-5 and C-6 as well as the steric environment at C-6. Treatment of II with methylguanidine gave 2-(methylamino)-4(3H)- pyrimidinone (59%) and 1-methylisocytosine (19%). II was also converted into uracil and 2-thiouracil by treatment with urea and thiourea, resp., in EtOH in the presence of EtONa. 1-Alkylated 2-thiouracils were obtained as the major products when II was treated with 1-methylthiourea or 1-n-butylthiourea. Treatment of II with excess 1,3-dimethylthiourea afforded 1,3-dimethyl-2-thiouracil. When II was treated with S-ethylthiuronium bromide, 2-(cyanoamino)-4(3H)-pyrimidinone was obtained. Treatment of II with formamidine, acetamidine, benzamidine, or 1,1-dimethylurea in base caused decomposition of the nucleophilic reagents, and unchanged II was recovered. Uracil, 1-methyluracil, or 3-methyluracil could not be converted into isocytosine by treatment with guanidine under various conditions. Application of this transformation reaction to 1,3-dimethylpseudouridine (III) gave the antileukemic agent, pseudoisocytidine (IV; R2 = H) in good yield when treated with guanidine. IV (R2 = Me) and 2-thiopseudouridine were also prepared by treatment of III with N-methylguanidine and thiourea, resp.
CC 33-7 (Carbohydrates)
Section cross-reference(s): 1, 63, 28

L79 ANSWER 22 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1970:445768 ZCAPLUS Full-text
DOCUMENT NUMBER: 73:45768
ORIGINAL REFERENCE NO.: 73:7563a,7566a

TITLE: Nucleosides. LXVII. Chemistry of 4-methyl-2-pyrimidinone ribonucleosides
AUTHOR(S): Klein, R. S.; Wempen, Iris; Watanabe, Kyoichi A.; Fox, Jack J.
CORPORATE SOURCE: Div. of Biol. Chem., Sloan-Kettering Inst. for Cancer Res., New York, NY, USA
SOURCE: Journal of Organic Chemistry (1970), 35(7), 2330-4
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI For diagram(s), see printed CA Issue.
AB The synthesis of 4-methyl-2-pyrimidinone ribonucleoside (I) and 4,5-dimethyl-2-pyrimidinone ribonucleoside (II) is described. The site of glycosylation is determined by two independent routes. Nitrosation of the 4-methyl group converts I and II into their corresponding oxime derivs. which, by treatment with Ac2O, afford the corresponding nitriles. The nitrile groups are easily displaced by a variety of nucleophiles. Reduction of the oxime from I followed by acetylation gives the N-acetylated aminomethyl derivative which undergoes facile air oxidation to the 4-carboxymethyl derivative (III). In model studies, the structure of III is established by an unambiguous synthesis of Me 1-methyl-2-oxo-4- pyrimidinecarboxylate (IV) from 3-methylorotic acid. 1-Methyl-2-oxo-4- pyrimidinecarboxaldehyde oxime is also shown to undergo reduction, acetylation, and autoxidn. to IV.
CC 33 (Carbohydrates)
ST pyrimidinone ribonucleosides; ribonucleosides pyrimidinone

L79 ANSWER 23 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1969:491418 ZCAPLUS Full-text
DOCUMENT NUMBER: 71:91418
ORIGINAL REFERENCE NO.: 71:17023a,17026a
TITLE: Pyrimidines. VIII. Direct nitration of monooxopyrimidines
AUTHOR(S): Wempen, Iris; Blank, H. Ulrich; Fox, Jack J.
CORPORATE SOURCE: Med. Coll., Sloan Kettering Inst. for Cancer Res., New York, NY, USA
SOURCE: Journal of Heterocyclic Chemistry (1969), 6(4), 593-5
CODEN: JHTCAD; ISSN: 0022-152X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 4- and 2-Oxopyrimidines are treated with KNO3 in H2SO4 at ≥90° to give 5-nitro-4-oxopyrimidine and 5-nitro-2-oxopyrimidine (I). The N.M.R. spectrum of the EtOH adduct of I is given.
CC 28 (Heterocyclic Compounds (More Than One Hetero Atom))
IT Nitration
(of pyrimidinones)

L79 ANSWER 24 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1969:58233 ZCAPLUS Full-text
DOCUMENT NUMBER: 70:58233
ORIGINAL REFERENCE NO.: 70:10961a,10964a
TITLE: 1-β-D-Arabinofuranosyl-5-fluorocytosines
INVENTOR(S): Fox, Jack Jay; Miller, Naishun C.
PATENT ASSIGNEE(S): Research Corp.
SOURCE: U.S., 3 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3404144	A	19681001	US 1965-516133	19651223
PRIORITY APPLN. INFO.:			US 1965-516133 A	19651223

GI For diagram(s), see printed CA Issue.

AB The title compds. (I), in which R1 and R2 are H, alkyl, alkenyl, aralkyl, cycloalkyl, or cycloalkenyl, are prepared by the action of R1R2NH on 1-β-D-arabinofuranosyl-5-fluoro-4-methylthio-2-pyrimidinone (II). 1-β-D-Arabinofuranosyl-5-fluorouracil (5.4 g.), 8 ml. Ac2O, and 60 ml. anhydrous C5H5N, 16 hrs. at room temperature addition of EtOH and evaporation of C5H5N, gave 7.78 g. 1-(tri-O-acetyl-β-D-arabinofuranosyl)-5-fluorouracil (III), m. 139-43° (50% EtOH), III (3.88 g.) was treated 3 times with 4.44 g. P2S5 for 4 hrs. in C5H5N. The solution was decanted and evaporated to dryness. Extraction with H2O, dissoln. of the residue in CH2Cl2, filtration, and evaporation gave 3 to 3.6 g. 1-(tri-O-acetyl-β-D- arabinofuranosyl)-5-fluoro-4-thiono-2-pyrimidinone (IV), yellow needles (MeOH), λmaximum 334, 224 nm. (50% EtOH). Methylation of IV in 250 ml. MeOH and 50 ml. H2O by 9 g. MeI, with addition of 34.5 ml. N NaOH during 40 min., neutralization by HOAc, and evaporation gave 87% II, m. 140-1° (H2O), [α]23D 219° (0.22, MeOH). II (5 g.) overnight in 25 ml. anhydrous NH3, evaporated, diluted with 50 ml. H2O, neutralized with HOAc, evaporated, and chromatographed on Dowex 50, gave 3.2 g. I, m. 237-8° (90% EtOH), [α]23D 163 ± 2° (0.18, H2O), pKa 2.33 ± 0.05. Oxidation of 0.3 g. 1-β-D-arabinofuranosyl-5-fluoro-4-thiono-2- pyrimidinone in 20 ml. phosphate buffer (pH 6.8) with 1.3 ml. N iodine solution gave 0.12 g. disulfide, m. 213-4° (50% EtOH). I is an anti-metabolite and has antiviral, antibacterial, antifungal, and antileukemic activity.

INCL 260211500

CC 33 (Carbohydrates)

L79 ANSWER 25 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1967:411696 ZCAPLUS Full-text

DOCUMENT NUMBER: 67:11696

ORIGINAL REFERENCE NO.: 67:2247a,2250a

TITLE: Nucleosides. XXXIX. 2'-Deoxy-2'-fluorocytidine, 1-β-D-arabinofuranosyl-2-amino-1,4(2H)-4-iminopyrimidine, and related derivatives

AUTHOR(S): Doerr, Iris L.; Fox, Jack J.

CORPORATE SOURCE: Sloan-Kettering Div. of Cornell Univ. Med. Coll., New York, NY, USA

SOURCE: Journal of Organic Chemistry (1967), 32(5), 1462-71
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB cf. CA 66: 76258y. Thiation of suitable protected 2'-deoxy-2'- halouridines followed by alkylation afforded 1-(2-deoxy-2-halo-β-D- ribofuranosyl)-4-methylthio-2-pyrimidinone (I) in good yields which, by treatment with liquid NH3, gave 2'-deoxy-2'-halocytidines (II) along with the halide salts (III, IV) of 1-β-D-arabinofuranosyl-2-amino-1,4(2H)- 4-iminopyrimidine. It is shown that in the above reaction of I, "aminoimino" nucleoside formed via intermediates II and 2,2'-anhydroarabinofuranosylcytosine (IV). The reaction of various 2,2'-anhydroarabinofuranosyl pyrimidines with liquid NH3 afforded 1-β-D-arabinofuranosyl derivatives of 5-methylisocytosine, 5-fluoroisocytosine, and 4-thioisocytosine. The hydrolytic reactions of 2'-deoxy-2'-halocytidines, 2,2'-anhydroarabinosylcytosine, and 2-aminopyrimidine nucleosides are reported and discussed.

CC 33 (Carbohydrates)

L79 ANSWER 26 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1966:473463 ZCAPLUS Full-text
DOCUMENT NUMBER: 65:73463
ORIGINAL REFERENCE NO.: 65:13698f-g
TITLE: Pyrimidines. VI. A novel degradation of 3-methyl-4thiouracil
AUTHOR(S): Watanabe, Kyoichi A.; Friedman, Herbert A.; Cushley, Robert J.; Fox, Jack J.
CORPORATE SOURCE: Cornell Univ. Med. Coll., New York, NY
SOURCE: Journal of Organic Chemistry (1966), 31(9), 2942-5
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 65:73463
AB cf. CA 62, 6481e. 3-Methyl-4-thiouracil (I) underwent an unexpected degradation when treated with dimethylamine in methanol at 155° 60 hrs. Three products were produced, two of which were identified as N,N-dimethylurea (II) and trans-β-dimethylaminothioacrylic acid methylamide (III). Catalytic reduction of III followed by N-methylation gave bis(1,3-dimethylamino)propane. Acid hydrolysis of the enamine III followed by catalytic reduction and then oxidation yielded β- methylaminopropionic acid. These chemical data along with N.M.R. studies establish structure III. The structure of I was confirmed by reduction to the known N-methyl-N,N'-trimethyleneurea. A plausible mechanism for the reaction of I → III and II via an isocyanate intermediate is proposed. 21 references.
CC 38 (Heterocyclic Compounds (More Than One Hetero Atom))
IT 10082-37-8P, Cyclopentaneacetic acid, 2-hydroxy-3-iodo-, γ-lactone
10082-42-5P, Cyclopentaneacetic acid, 2-hydroxy-α-(ureidomethylene)-, γ-lactone 10082-43-6P, Cyclopentaneacetic acid, 2-hydroxy-α-[(thioureido)methylene]-, γ-lactone 10082-60-7P, 1,3-Propanediamine, N,N,N',N'-tetramethyl-, dihydrochloride 35389-45-8P, 1,3-Propanediamine, N,N,N',N'-tetramethyl-, dipicrate 90873-48-6P, 4(3H)-Pyrimidinone, 5-(2-hydroxycyclopentyl)-2-(methylthio)-
91176-88-4P, Cyclopentaneacetic acid, 2-hydroxy-α-(hydroxymethylene)-, γ-lactone 843613-83-2P, Cyclopentaneacetic acid, 2-hydroxy-, (±)-cis-
RL: PREP (Preparation)
(preparation of)

L79 ANSWER 27 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1966:44135 ZCAPLUS Full-text
DOCUMENT NUMBER: 64:44135
ORIGINAL REFERENCE NO.: 64:8285g-h,8286a-b
TITLE: Nucleosides. XXXI. 3'-Amino-3'-deoxyhexopyranosyl nucleosides. 4. Nucleoside conversions in the 3'-aminohexose series
AUTHOR(S): Watanabe, Kyoichi A.; Fox, Jack J.
CORPORATE SOURCE: Sloan-Kettering Inst. for Cancer Res., New York, NY
SOURCE: Journal of Organic Chemistry (1966), 31(1), 211-17
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 64:44135
GI For diagram(s), see printed CA Issue.
AB 1-(3-Amino-3-deoxy-β-D-mannopyranosyl)- uracil was prepared from its D-gluco isomer in a 7-step synthesis proceeding via 1-(3-acetamido-3-deoxy- 2-O-methylsulfonyl-4,6-O-benzylidene-β-D-glucosyl)uracil (I). I was converted to the 2,2'-anhydro derivative (II), the first of its kind in the hexopyranosyl

nucleoside area. The structure II was established by its conversion to 1-(3-acetamido-3-deoxy-4,6-O-benzylidene-β-D- mannosyl)isocytosine with liquid NH3 and to 1-(3-acetamido-3-deoxy-4,6-O- benzylidene-β-D-mannosyl)uracil with alkali, the latter of which, after removal of blocking groups, yielded III. An attempted conversion of IV to V via the aziridine (VI) was carried out. Some indication of formation of V was obtained along with the formation of the crystalline hydrochloride of 1-(3-amino-3-deoxy-β-D-galactopyranosyl)uracil. The latter nucleoside was also obtained directly from uridine by the periodate-MeNO2 procedure. Cf. J. Med. Chemical 9(1), 101-5(1966); CA 63, 13382b.

CC 43 (Carbohydrates)

IT 6205-98-7P, Uracil, 1-(3-acetamido-4,6-O-benzylidene-3-deoxy-β-D-glucopyranosyl)- 6205-99-8P, Uracil, 1-(3-amino-3-deoxy-β-D-mannopyranosyl)-, hydrochloride 6206-00-4P, Uracil, 1-(3-acetamido-4,6-O-benzylidene-3-deoxy-β-D-glucopyranosyl)-, 2'-methanesulfonate 6206-02-6P, Uracil, 1-(3-acetamido-4,6-O-benzylidene-3-deoxy-β-D-mannopyranosyl)- 6206-03-7P, Uracil, 1-(3-amino-3-deoxy-β-D-galactopyranosyl)-, hydrochloride 6206-04-8P, Uracil, 1-(3-acetamido-3-deoxy-β-D-glucopyranosyl)-, 2'-acetate 6206-05-9P, Uracil, 1-(3-acetamido-3-deoxy-6-O-trityl-β-D-glucopyranosyl)-, 2'-acetate 6206-06-0P, Uracil, 1-(3-acetamido-3-deoxy-6-O-trityl-β-D-glucopyranosyl)-, 2'-acetate 4'-methanesulfonate 6414-66-0P, Uracil, 1-(3-acetamido-4,6-O-benzylidene-3-deoxy-β-D-glucopyranosyl)-, 2'-acetate 99800-56-3P, 4(1H)-Pyrimidinone, 1-(3-acetamido-4,6-O-benzylidene-3-deoxy-β-D-mannopyranosyl)-
RL: PREP (Preparation)
(preparation of)

L79 ANSWER 28 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1966:52330 ZCAPLUS Full-text
DOCUMENT NUMBER: 64:52330
ORIGINAL REFERENCE NO.: 64:9809c-d
TITLE: Nucleosides. XXIX. 1-β-D-Arabinofuranosyl-5-fluorocytosine and related arabino nucleosides
AUTHOR(S): Fox, Jack J.; Miller, Naishun; Wempen, Iris
CORPORATE SOURCE: Sloan-Kettering Inst. for Cancer Res., New York, NY
SOURCE: Journal of Medicinal Chemistry (1966), 9(1), 101-5
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 64:52330

AB cf. CA 63, 13382b. Reaction of the 5'-O-trityl derivative of uridine or 5-fluorouridine with thiocarbonyldiimidazole yielded crystalline 2,2'-anhydro-1-(β-D-arabinofuranosyl)uracils directly in high yields. These derivs. were converted to 1-β-D-arabinofuranosyluracil and 1-β-D-arabinofuranosyl-5-fluorouracil (FUA) in high yield. FUA was acetylated, thiated, and then alkylated to the 4-methylthio derivative which was converted with liquid NH3 to 1-β-D-arabinofuranosyl-5- fluorocytosine (FCA). FUA, FCA, and 1-β-D-arabinofuranosylcytosine (CA) were active against Sarcoma 180 in mice. FCA was highly active against transplanted mouse leukemias P815 and P388, and FCA was more strongly active on a molar basis than CA against a 5-fluorouracil-resistant line of mouse leukemia P815. FCA and CA were effective against the 5-fluorouracil-resistant L1210 mouse leukemia. FCA, CA, and IUDR showed essentially the same activity in preventing the development of herpes keratitis in rabbits.

CC 43 (Carbohydrates)

IT 131-06-6P, Uracil, 1-β-D-arabinofuranosyl-5-fluoro- 3736-77-4P,

6H-Furo[2',3':4,5]oxazolo[3,2-a]pyrimidin-6-one, 2,3,3a,9a-tetrahydro-3-hydroxy-2-(hydroxymethyl)- 4298-10-6P, Cytosine, 1-β-D-arabinofuranosyl-5-fluoro- 6160-58-3P, Uracil, 1-(5-O-trityl-β-D-arabinofuranosyl)- 6160-60-7P, Uracil, 5-fluoro-1-(5-O-trityl-β-D-arabinofuranosyl)- 6160-61-8P, Uracil, 1-β-D-arabinofuranosyl-5-fluoro-, 2',3',5'-triacetate 6160-62-9P, Uracil, 1-β-D-arabinofuranosyl-5-fluoro-4-thio-, 2',3',5'-triacetate 6160-63-0P, 2(1H)-Pyrimidinone, 1-β-D-arabinofuranosyl-5-fluoro-4-(methylthio)- 6160-65-2P, Imidazole, 1,1'-(thiocarbonyl)di- 6412-18-6P, 2(1H)-Pyrimidinone, 4,4'-dithiobis[1-β-D-arabinofuranosyl-5-fluoro- 187592-53-6P, Uracil, 2,2'-anhydro-5-fluoro-1-(5'-O-trityl-β-D-arabinofuranosyl)-
RL: PREP (Preparation)
(preparation of)

L79 ANSWER 29 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1964:496257 ZCAPLUS Full-text
DOCUMENT NUMBER: 61:96257
ORIGINAL REFERENCE NO.: 61:4345f-g
TITLE: Pyrimidines. IV. The interconversion of N4-methylcytosine and 3-methylcytosine
AUTHOR(S): Ueda, Tohru; Fox, Jack J.
CORPORATE SOURCE: Cornell Univ. Med. Coll., New York, NY
SOURCE: J. Org. Chem. (1964), 29(7), 1770-2
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB N4-Methylcytosine (I), when refluxed with Ac2O-AcOH for prolonged periods, rearranges to 3-methylcytosine (II). The reversibility of this reaction is shown, and a mechanism for the rearrangement is given.
CC 38 (Heterocyclic Compounds (More Than One Hetero Atom))
IT 2950-82-5P, 1(2H)-Pyrimidinepropionic acid, 3,4-dihydro-2,4-dioxo- 7329-75-1P, Cytosine, N-acetyl-1-methyl- 17994-74-0P, 1(6H)-Pyrimidinepropionitrile, 2-(methylthio)-6-oxo- 35886-91-0P, Butyric acid, 4-[(1,2-dihydro-2-oxo-4-pyrimidinyl)-amino]- 89852-95-9P, 1(2H)-Pyrimidinepropionitrile, 4-amino-2-oxo- 89854-00-2P, 1(2H)-Pyrimidinepropionic acid, 6-amino-2-oxo 90091-18-2P, 1(2H)-Pyrimidinepropionic acid, 6-amino-α-methyl-2-oxo- 90151-21-6P, 1(2H)-Pyrimidinepropionic acid, 3,6-dihydro-2,6-dioxo- 90223-17-9P, 2(1H)-Pyrimidinone, 4-(2-oxo-1-pyrrolidinyl)- 90438-19-0P, 1(2H)-Pyrimidinepropionic acid, 3,6-dihydro-2,6-dioxo-, ethyl ester 90607-50-4P, Alanine, N-(1,2-dihydro-2-oxo-4-pyrimidinyl)-2-methyl- 90607-51-5P, β-Alanine, N-(1,2-dihydro-1-methyl-2-oxo-4-pyrimidinyl)- 90872-26-7P, β-Alanine, N-acetyl-N(1,2-dihydro-1-methyl-2-oxo-4-pyrimidinyl)- 91724-59-3P, 2H-Pyrimido[1,6-a]pyrimidine-2,6(1H)-dione, 3,4-dihydro- 91847-04-0P, Cytosine, N-acetyl-N-methyl- 91996-64-4P, Imidazo[1,2-c]pyrimidine-2,5(1H,3H)-dione, 3-methyl- 92660-40-7P, Imidazo[1,2-c]pyrimidine-2,5(1H,3H)-dione, 3,3-dimethyl- 92660-53-2P, 2H-Pyrimido[1,6-a]pyrimidine-2,6(1H)-dione, 3,4-dihydro-3-methyl- 93263-10-6P, 1(2H)-Pyrimidinepropionic acid, 6-amino-2-oxo-, ethyl ester, hydrochloride
RL: PREP (Preparation)
(preparation of)

L79 ANSWER 30 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1964:425388 ZCAPLUS Full-text
DOCUMENT NUMBER: 61:25388
ORIGINAL REFERENCE NO.: 61:4345d-f
TITLE: Pyrimidines. III. A novel rearrangement in the

syntheses of imidazo- or pyrimidol[1,2-c]pyrimidines
AUTHOR(S): Ueda, Tohru; Fox, Jack J.
CORPORATE SOURCE: Cornell Univ. Med. Coll., New York, NY
SOURCE: Journal of Organic Chemistry (1964), 29(7), 1762-9
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 61:25388
GI For diagram(s), see printed CA Issue.
AB cf. CA 60, 12007g. Pyrimidinylamino acids [e.g., N-(1H-2-oxo-4- pyrimidinyl)-β-alanine (I)] treated with Ac2O cyclized with rearrangement to 2-oxopyrimido- or 2-oxoimidazo[1,2-c]pyrimidines, e.g. II or III. This novel rearrangement occurred with pyrimidinyl-α or -β simple amino acid derivs. A mechanism was given which involved the cleavage of the C2-N3 linkage of the pyrimidine ring of I with formation of an amide linkage between the carboxyl group of the amino acid moiety and N3 to form IV. Recyclization occurs between C2 and N4 of intermediate IV to furnish II. The presence of H on N1 of the pyrimidinyl amino acids was essential for the rearrangement. N1-Alkylated pyrimidinyl amino acids does not undergo the rearrangement; instead other reactions predominate. γ-Amino acid derivs. yield N-4- pyrimidinylbutyrolactams(35).
CC 38 (Heterocyclic Compounds (More Than One Hetero Atom))
IT 2950-82-5P, 1(2H)-Pyrimidinepropionic acid, 3,4-dihydro-2,4-dioxo- 7329-75-1P, Cytosine, N-acetyl-1-methyl- 17994-74-0P, 1(6H)-Pyrimidinepropionitrile, 2-(methylthio)-6-oxo- 35886-91-0P, Butyric acid, 4-[(1,2-dihydro-2-oxo-4-pyrimidinyl)-amino]- 89852-95-9P, 1(2H)-Pyrimidinepropionitrile, 4-amino-2-oxo- 89854-00-2P, 1(2H)-Pyrimidinepropionic acid, 6-amino-2-oxo- 90091-18-2P, 1(2H)-Pyrimidinepropionic acid, 6-amino-α-methyl-2-oxo- 90151-21-6P, 1(2H)-Pyrimidinepropionic acid, 3,6-dihydro-2,6-dioxo- 90223-17-9P, 2(1H)-Pyrimidinone, 4-(2-oxo-1-pyrrolidinyl)- 90438-19-0P, 1(2H)-Pyrimidinepropionic acid, 3,6-dihydro-2,6-dioxo-, ethyl ester 90607-48-0P, Alanine, N-(1,2-dihydro-1-methyl-2-oxo-4-pyrimidinyl)-, (±)- 90607-50-4P, Alanine, N-(1,2-dihydro-2-oxo-4-pyrimidinyl)-2-methyl- 90607-51-5P, β-Alanine, N-(1,2-dihydro-1-methyl-2-oxo-4-pyrimidinyl)- 90607-52-6P, β-Alanine, N-(1,2-dihydro-2-oxo-4-pyrimidinyl)-2-methyl-, ±- 90872-26-7P, β-Alanine, N-acetyl-N(1,2-dihydro-1-methyl-2-oxo-4-pyrimidinyl)- 91724-59-3P, 2H-Pyrimido[1,6-a]pyrimidine-2,6(1H)-dione, 3,4-dihydro- 91847-04-0P, Cytosine, N-acetyl-N-methyl- 91996-64-4P, Imidazo[1,2-c]pyrimidine-2,5(1H,3H)-dione, 3-methyl- 92660-40-7P, Imidazo[1,2-c]pyrimidine-2,5(1H,3H)-dione, 3,3-dimethyl- 92660-53-2P, 2H-Pyrimido[1,6-a]pyrimidine-2,6(1H)-dione, 3,4-dihydro-3-methyl- 93117-34-1P, Imidazo[1,2-c]pyrimidin-5(1H)-one, 2-hydroxy-3-methyl-, acetate (ester) 93263-10-6P, 1(2H)-Pyrimidinepropionic acid, 6-amino-2-oxo-, ethyl ester, hydrochloride 93738-70-6P, Imidazo[1,2-c]pyrimidin-5-(6H)-one, 3-hydroxy-2,6-dimethyl-, acetate (ester) 96117-01-0P, Imidazo[1,2-c]pyrimidin-5-(6H)-one, 3-hydroxy-2,6-dimethyl-, acetate (ester), acetate 96984-45-1P, Imidazo[1,2-c]pyrimidin-5(1H)-one, 1-acetyl-2-hydroxy-3-methyl-, acetate (ester) 857021-26-2P, Cytosine, N-methyl-, 3-methylcytosine
RL: PREP (Preparation)
(preparation of)

L79 ANSWER 31 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1964:23386 ZCAPLUS Full-text
DOCUMENT NUMBER: 60:23386
ORIGINAL REFERENCE NO.: 60:4140h,4141a-b
TITLE: Spectrophotometric studies of nucleic acid derivatives and related compounds. V. Structure of

3-methylcytosine
AUTHOR(S): Ueda, Tohru; Fox, Jack J.
CORPORATE SOURCE: Cornell Univ. Med. Coll., New York, NY
SOURCE: Journal of the American Chemical Society (1963), 85(24), 4024-8
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
GI For diagram(s), see printed CA Issue.
AB cf. CA 51 10540h. Several 2,3-dihydroimidazo[1,2-c]pyrimidines were synthesized by reaction of 4-thiouracil or 4-methylthio-2-pyrimidinone or 1-methyl-4-methylthio-2-pyrimidinone with amino alcs. followed by chlorination and ring closure to condensed-ring systems. The absorption spectra of these compds. were determined and their dissociation consts. measured spectrally. Spectral comparisons of appropriate mol. species showed that the structure of 3-methylcytosine (neutral species) is of the 4-amino-2-oxo form. 3-Methylcytosine exhibits a hitherto unreported 2nd dissociation (as demonstrated spectrally) in the high alkaline region attributable to proton removal from the 4-amino group. The difference in pKa1 values between 1-alkylated and 3-alkylated cytosines is explained by the difference in basicity of their site of protonation. A 1,2,3,4-tetrahydropyrimido[1,2-c]pyrimidine (I), a new ring system, was also synthesized.
CC 38 (Heterocyclic Compounds (More Than One Hetero Atom))

L79 ANSWER 32 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1963:482495 ZCAPLUS Full-text
DOCUMENT NUMBER: 59:82495
ORIGINAL REFERENCE NO.: 59:15376h,15377a-b
TITLE: Pyrimidine nucleosides. XVII. Pyrimidinyl amino acids
AUTHOR(S): Ueda, Tohru; Fox, Jack J.
CORPORATE SOURCE: Cornell Univ. Med. Coll., New York, NY
SOURCE: Journal of Medicinal Chemistry (1963), 6(6), 697-701
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 59:82495
GI For diagram(s), see printed CA Issue.
AB cf. CA 58, 11457a. N-(2-Oxo-4-pyrimidinyl) amino acids were prepared by reaction of 4-methylthio-2-pyrimidinones with amino acids. N-(2Oxo-4-pyrimidinyl)glycine, -L-alanine, -L-phenylalanine (I), -L-ryptophan (II), -β-alanine, -o- and p-amiuobenzoic acid (III), and -glycylglycine were obtained. N-(2-Thio-4-pyrimidinyl)-L-tryptophan was also prepared as well as the 5-methyl, 5-fluoro (IV), 5-chloro, and 5-bromo analogs of N-(2-oxo-4-pyrimidinyl)-DL-alanine. The ribonucleosides of I, II, and III were synthesized by treatment of 1-β-D-ribofuranosyl-4- methylthio-2-pyrimidinone with the appropriate amino acid. The 1-(2-deoxy-β-D-ribofuranosyl) derivative of IV was synthesized by similar methods. Preliminary results with some of these compds. in exptl. tumors showed no significant antitumor activity. None of the pyrimidinyl amino acids tested supported the growth of certain pyrimidine- or amino acid-requiring mutants of Escherichia coli.
CC 44 (Amino Acids, Peptides, and Proteins)
IT 671-41-0P, Uracil, 5-fluoro-4-thio- 1480-95-1P, 2(1H)-Pyrimidinone, 5-fluoro-4-(methylthio)- 14795-38-1P, 2(1H)-Pyrimidinone, 4-(methylthio)-1-β-D-ribofuranosyl- 19674-84-1P, Glycine, N-(1,2-dihydro-2-oxo-4-pyrimidinyl)- 28279-68-7P, Alanine, N-(1,2-dihydro-2-oxo-1-β-D-ribofuranosyl-4-pyrimidinyl)-3-phenyl-, L- 42497-06-3P, Glycine, N-[N-(1,2-dihydro-2-oxo-4-pyrimidinyl)-glycyl]- 49844-93-1P, Pyrimidine, 2-chloro-4-(methylthio)- 51674-12-5P, 2(1H)-Pyrimidinethione, 4-(methylthio)- 55040-79-4P, 2(1H)-

Pyrimidinone, 5-methyl-4-(methylthio)- 64988-60-9P, Anthranilic acid, N-(1,2-dihydro-2-oxo-4-pyrimidinyl)- 89641-68-9P, Pseudourea, 2-thio-, compound with 4-(methylthio)-2(1H)-pyrimidinethione 89641-68-9P, 2(1H)-Pyrimidinethione, 4-(methylthio)-, compound with 2-thiopseudourea 89853-89-4P, β-Alanine, N-(1,2-dihydro-2-oxo-4-pyrimidinyl)- 89886-00-0P, Alanine, N-(5-fluoro-1,2-dihydro-2-oxo-4-pyrimidinyl)-, L- 90000-81-0P, Alanine, N-(1,2-dihydro-2-oxo-4-pyrimidinyl)-, DL- 90000-81-0P, Alanine, N-(1,2-dihydro-2-oxo-4-pyrimidinyl)-, L- 91093-56-0P, Benzoic acid, p-[(1,2-dihydro-2-oxo-4-pyrimidinyl)amino]- 93003-52-2P, Alanine, N-(1,2-dihydro-2-oxo-4-pyrimidinyl)-3-phenyl-, L- 93312-34-6P, Benzoic acid, p-[(1,2-dihydro-2-oxo-1-β-D-ribofuranos-yl-4-pyrimidinyl)amino]- 93734-56-6P, Tryptophan, N-(1,2-dihydro-2-thioxo-4-pyrimidinyl)- 93734-66-8P, Tryptophan, N-(1,2-dihydro-2-oxo-4-pyrimidinyl)- 95556-24-4P, Tryptophan, N-(1,2-dihydro-2-oxo-1-β-D-ribofuranosyl-4-pyrimidinyl)-, L- 95769-92-9P, 2(1H)-Pyrimidinone, 1-(2-deoxy-β-D-erythro-pentofuranosyl)-5-methyl-4-(methylthio)- 887229-93-8P, Alanine, N-(5-chloro-1,2-dihydro-2-oxo-4-pyrimidinyl)-, L- 887229-97-2P, Alanine, N-(1,2-dihydro-5-methyl-2-oxo-4-pyrimidinyl)-, L- 887230-32-2P, Alanine, N-[1-(2-deoxy-β-D-erythropentofuranosyl)-5-fluoro-1,2-dihydro-2-oxo-4-pyrimidinyl]-, L- 887231-77-8P, Alanine, N-(5-bromo-1,2-dihydro-2-oxo-4-pyrimidinyl)-, L-
RL: PREP (Preparation)
(preparation of)

L79 ANSWER 33 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1963:482241 ZCAPLUS Full-text
DOCUMENT NUMBER: 59:82241
ORIGINAL REFERENCE NO.: 59:15274b-c
TITLE: Pyrimidines. I. The synthesis of 6-fluorocytosine and related compounds
AUTHOR(S): Wempen, Iris; Fox, Jack J.
CORPORATE SOURCE: Cornell Univ. Med. Coll., New York, NY
SOURCE: Journal of Medicinal Chemistry (1963), 6(6), 688-93
CODEN: JMCMAR; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 59:82241
GI For diagram(s), see printed CA Issue.
AB Syntheses of 6-fluorocytosine (I) and 6-fluoroisocytosine from 2,4,6-trifluoropyrimidine and the preparation of a number of mono- and difluoropyrimidine intermediates are described. 5-Chlorocytosine and 5-chloroisocytosine were obtained from cytosine or isocytosine by use of N-chlorosuccinimide in AcOH. The relative effects of a 5- and 6-halo atom on the ultraviolet absorption spectra and apparent pK8 values of cytosine and isocytosine are presented.
CC 38 (Heterocyclic Compounds (More Than One Hetero Atom))
IT 658-87-7P, Pyrimidine, 4-fluoro-2,6-dimethoxy- 675-11-6P, Pyrimidine, 2-amino-4,6-difluoro- 675-12-7P, Pyrimidine, 4-amino-2,6-difluoro- 696-83-3P, Pyrimidine, 2,4-diamino-6-fluoro- 701-67-7P, Pyrimidine, 2-amino-4-ethoxy-6-fluoro- 722-16-7P, Pyrimidine, 2-amino-4-(benzyloxy)-6-fluoro- 722-17-8P, Pyrimidine, 4-amino-2-(benzyloxy)-6-fluoro- 1194-21-4P, 4(3H)-Pyrimidinone, 2-amino-6-chloro- 1683-86-9P, 4(3H)-Pyrimidinone, 2-amino-5-fluoro- 2022-85-7P, Cytosine, 5-fluoro- 2193-47-7P, Cytosine, 6-fluoro- 2240-25-7P, Cytosine, 5-bromo- 2253-05-6P, 4(3H)-Pyrimidinone, 2-amino-6-fluoro- 2347-43-5P, Cytosine, 5-chloro- 3289-35-8P, Cytosine, 6-chloro- 3289-50-7P, Pyrimidine, 4-amino-2,6-dimethoxy- 31458-45-4P, 2(1H)-Pyrimidinone, 4,6-diamino- 36315-01-2P, Pyrimidine, 2-amino-4,6-dimethoxy- 42956-82-1P, 4-Pyrimidinol, 2-amino-6-ethoxy-

61937-71-1P, 4(3H)-Pyrimidinone, 2-amino-5-bromo- 89033-81-8P, 4(3H)-Pyrimidinone, 2-amino-5-chloro- 90843-04-2P, Pyrimidine, 2,4,6-triamino-, picrate 143504-99-8P, 4(3H)-Pyrimidinone, 2,6-diamino-
RL: PREP (Preparation)
(preparation of)

L79 ANSWER 34 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1962:31420 ZCAPLUS Full-text
DOCUMENT NUMBER: 56:31420
ORIGINAL REFERENCE NO.: 56:5960h-i,5961a-g
TITLE: Pyrimidine nucleosides. XII. Direct synthesis of 2'-deoxycytidine and its α-anomer
AUTHOR(S): Fox, Jack F.; Yung, Naishun; Wempen, Iris; Hoffer, Max
CORPORATE SOURCE: Hoffmann La Roche, Inc., Nutley, NJ
SOURCE: Journal of the American Chemical Society (1961), 83, 4066-50
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 56:31420

AB The direct synthesis of 2'-deoxycytidine (I) was achieved via the mercuri method involving the condensation of 3,5 di-O-(p-chlorobenzoyl)-2-deoxy-D-ribosyl chloride (II) with mercuri-N-acetylcytosine (III). The α-anomer (IV) of I was also obtained from this reaction. The synthesis of II from 2-deoxy-D-ribose (V) was described. The optical rotations of I and IV, as well as those of their acylated intermediates, did not conform to Hudson's rules of isorotation. The synthesis of other fully acylated derivs. of 2-deoxy-D-ribofuranose from preformed purine-2-deoxy-D-ribonucleosides also was described. V (20.0 g.) in 380 cc. absolute MeOH treated 20 min. at 27° with 20 cc. 1% HClMeOH, stirred with 10.0 g. Ag2CO3, filtered and evaporated, the residue dissolved in C5H5N, concentrated, and dissolved in 115 cc. dry C5H5N, the solution treated 16 hrs. with cooling with 45 cc. p-ClC6H4COCl and diluted with H2O and CH2Cl2, the organic layer worked up, and the sirupy Me 3,5-di-O-(p-chlorobenzoyl)-2- deoxy-D-ribofuranoside dissolved in 150 cc. dry Et2O, cooled to 0°, treated with 200 cc. cold AcOH (saturated with dry HCl), saturated below 10° with dry HCl, and filtered gave 28.0 g. II, m. 118-20° (decomposition). II (0.005 mole) added with stirring to 0.0025 mole dry III in 40 cc. refluxing xylene, cooled, filtered, and diluted with 300 cc. petr. ether and the precipitate purified gave 0.8 g. 1-[3,5-di-O-(p-chlorobenzoyl)-2- deoxy-α-D-ribosyl]-4-acetamido-2(1H)-pyrimidinone (VI) and β-anomer; the mother liquor gave 0.1 g. unidentified, N-free, crystalline material, m. about 160°. α-and β-VI mixture (0.8 g.) in about 20 cc. hot EtOH when cooled deposited about 0.3 g. α-VI, needles, m. 200-1° with sintering at about 160°, resolidifying, and remelting with effervescence at about 230°; this material recrystd. from about 25 cc. boiling EtOH gave short needles, m. 204.5-205°, becoming turbid at 208°, resolidifying at 210°, and remelting with decomposition at about 245°, [α]25D -66° (c 0.9, CHCl3); the mother liquor from the α-VI concentrated to 10 cc. and cooled gave 0.44 g. β-VI, m. 128-30° (hot EtOH), resolidifying and remelting with decomposition and effervescence at about 240°, [α]25D -19° (c 0.9, CHCl3). α-VI (250 mg.) in 30 cc. absolute EtOH (saturated at 0° with dry NH3) heated 12 hrs. at 100° in a sealed tube and worked up gave 100 mg. IV, m. 192-3° (EtOH), [α]25D -44° (c 0.7, N NaOH); picrate, microscopic prisms, m. 173-5° (decomposition and effervescence) (95% EtOH). β-VI (300 mg.) gave similarly I, m. 199-200° (MeOH and Et2O); picrate, yellow needles, m. 192-8°. Deoxyadenosine (20.1 g.) dissolved with stirring in about 750 cc. dry C5H5N, cooled, treated with stirring dropwise with 28 cc.

BzCl, kept 48 hrs. at 37-9°, concentrated in vacuo to about 200 cc., and stirred into about 200 cc. ice and H2O, and the aqueous layer decanted gave 37 g. glassy solid; the product heated 2 hrs. with stirring on the steam bath with 1700 cc. 2N H2SO4 and 500 cc. Bu2O, the aqueous layer again refluxed 1 hr. with 500 cc. Bu2O, and the combined organic phases cooled, filtered, and worked up gave 19 g. 3,5-di-O-benzoyl-D-ribose (VII). 2'-Deoxyguanosine benzoylated in a similar manner and the product dissolved in dioxane and refluxed with Bu2O and 2N H2SO4 gave 65% VII. VII (0.056 mole) in 60 cc. dry C5H5N and 80 cc. CH2Cl2 treated 2 days at room temperature with 17.1 g. Ac2O, evaporated below 50° in vacuo, poured into iced H2O, and extracted with CHCl3, and the extract worked up yielded 22% (crude) 1-O-acetyl-3,5-di-O-benzoyl-2-deoxy-D-ribose, m. 86.5-7.5° (EtOH), [α]26D -23° (c 2.0, CHCl3). VII benzoylated in a similar manner gave 15% 1,3,5-tri-O-benzoyl-2-deoxy-D-ribose, needles, m. 110-11° (EtOH), [α]25D 75° (c 2.54, CHCl3); the original mother liquor yielded 7% of an isomer, needles, m. 83-6° (EtOH), [α]25D -20° (c 1.1, CHCl3). The infrared absorption spectra of I and IV were recorded.

CC 32 (Heterocyclic Compounds-More than One Hetero Atom)

L79 ANSWER 35 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1961:93507 ZCAPLUS Full-text
DOCUMENT NUMBER: 55:93507
ORIGINAL REFERENCE NO.: 55:17640f-i,17641a-f
TITLE: Pyrimidine nucleosides. VIII. Synthesis of 5-nitrocytidine and related nucleosides
AUTHOR(S): Fox, Jack J.; Van Praag, Dina
CORPORATE SOURCE: Sloan-Kettering Inst. for Cancer Research, New York, NY
SOURCE: Journal of Organic Chemistry (1961), 26, 526-32
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. CA 54, 24764i. The Hg reaction for pyrimidine nucleoside synthesis was extended to 5-nitrocytosine (I). Condensation of bis(5- nitrocytosine)mercury (II) with poly-O-acylglycosyl halides yielded nucleosides in which the sugar moiety was linked to the pyrimidine at position 1. Reduction of the 5-nitro group of these nucleosides (e.g., I) afforded 5-amino analogs, which were cyclized to 1-β-D-glycosyl-2- oxopurines or their corresponding 8-aza analogs. Modifications were given for the synthesis of 1-methyl- (III) and 9-methyl-2-oxopurine (IV) and some of the intermediates used in their preparation 2-Oxo-8-azapurine (V) was synthesized by treatment of 5-aminocytosine (VI) with HNO2. Ultraviolet absorption spectra and spectrally determined pKa values for key compds. in the above syntheses were given. I (46.8 g.) suspended in 700 ml. hot H2O and 300 ml. N NaOH treated slowly with an alc. solution of 40.5 g. HgCl2 gave 76.5 g. II.H2O. II (27 g.) suspended in 1200 ml. PhMe dried azeotropically and 0.1 mole tetra-O-acetyl-β-D-glucopyranosyl bromide added in 2 portions and the mixture refluxed 2 hrs., concentrated, and treated with ligroine gave 40 g. 1-(tetra-O-acetyl-β-D-glucopyranosyl)-5- nitrocytosine (VII), m. 220-2° (MeOH). VII (9.7 g.) suspended in 400 ml. MeOH and 150 ml. AcOH shaken 23 min. at room temperature under H with 5 g. 5% Pd-C gave 8.3 g. 1-(tetra-O-acetyl-β-D-glucopyranosyl)-5- aminocytosine (VIII), m. 274-5° (alc.). VIII (5.46 g.) refluxed 1 hr. in 25 ml. AcOCH(OEt)2 gave 3.9 g. 1-(tetra-O-acetyl-β-D- glucopyranosyl)-2-oxopurine (IX), m. 284-5°. IX (4.7 g.) in MeOH treated 1 day at room temperature with 100 ml. alc. NH3 gave 2.6 g. 1-(β-D-glucopyranosyl)-2-oxopurine (X), m. 285-90°, [α]25D 57° (c 0.7, H2O). VII (3 g.) in 250 ml. alc. NH3 shaken 1 hr. at room temperature, left 3 days at room temperature, and the residue crystallized gave 0.8 g. 1-(β-D-glucopyranosyl)-5-nitrocytosine, m. 243-5° (alc.). 1-O-Acetyl-2,3,5-tri-O-benzoyl-D-ribose (0.04 mole) in 600 ml. Et2O saturated at 0° with HCl, left 3-

5 days, resatd. at 0° with HCl, and left 1 day longer, and the 2,3,5-tri-O-benzoyl-D- ribofuranosyl chloride in PhMe added to 0.02 mole II in 200 ml. PhMe, the mixture distilled to remove H2O, evaporated to half volume, the concentrate poured into 1500 ml. ligroine, the mixture cooled, filtered, the precipitate taken up in -CHCl3, and the solution washed with 300 ml. 30% KI and evaporated gave 19.6 g. 1-(tri-O-benzoyl-β-D-ribofuranosyl)-5-nitrocytosine (XI), m. 218-19°, [α]25D -133° (c 0.2, CHCl3). XI (6 g.), suspended in 150 ml. 80% alc., treated with N NaOH 2 hrs. at room temperature gave 2.8 g. 5-nitrocytidine (XII), shrinking at .apprx.120°, brown at .apprx.150°, and blackening at 175-300°, [α]25D -21° (c 0.7, H2O). XII in hot H2O kept 24 hrs. with excess HCl and NaNO2, addnl. HCl and NaNO2 added, and after several days at room temperature the mixture chromatographed on Schuell paper gave one spot corresponding to that for 5-nitrouridine. XII (3.3 g.) and 3.3 g. 5% Pd-C suspended in 300 ml. MeOH containing 5 ml. AcOH shaken 5 min. at room temperature under H gave 2.2 g. 5-aminocytidine (XIII), m. 211-12° (decomposition) (MeOH-H2O), [α]25D 4° (c 2.7, H2O); HCl salt, brown at .apprx.175°, blackening at .apprx.190°, not melting below 320°; sulfate salt decomposing 212°. XIII or its HCl salt (2 g.) refluxed 3 hrs. at 120° in 20 ml. AcOCH(OEt)2 gave 0.95 g. 1-β-D-ribofuranosyl-2-oxopurine, m. 207-8° (H2O), [α]25D 93° (c 0.7, H2O). XIII (1.29 g.) or its HCl salt in 2.5 ml. 2N HCl treated with 0.340 g. NaNO2 at 0-5° gave 1 g. 5-oxo-6-(β-D- ribofuranosyl)-1H-v-triazolo[4,5-d] pyrimidine, [α]25D 50° (c 0.23, H2O). Nitration of 0.26 g. 1-methylcytosine in 1 ml. concentrated H2SO4 treated gradually with 0.66 ml. fuming HNO3 gave 1-methyl-5-nitrocytosine (XIV), m. 271-3°. XIV (4 g.) and 2 g. Pd-C suspended in 450 ml. H2O and shaken at room temperature with H gave 0.4 g. 1-methyl-5-aminocytosine (XIVa), decomposing above 220°. 4-Ethoxy-2(1H)-pyrimidinone (2 g.) and 40 ml. 30% alc.-MeNH2 heated 12 hrs. at 120° in a sealed tube gave 1.4 g. 4-methylamino-2(1H)-pyrimidinone (XV), m. .apprx.270° (decomposition) (dilute alc.). XV suspended in H2O with Pd-C and shaken with H gave 45% 4-methylamino-5-amino-2(1H)-pyrimidinone (XVI), decomposing 220°. XVI (0.45 g.) refluxed 2 hrs. in 5 ml. AcOCH(OEt)2 gave 0.25 g. IV, m. 305-6° (decomposition) (H2O-NH4OH). XIVa (1 g.) heated 1 hr. at 120-30° with 20 ml. AcOCH(OEt)2 gave 0.6 g. III, decomposing above 280° (H2O). I (1.5 g.) reduced as above gave 0.9 g. VI, no definite decomposition point. VI (1.1 g.) in 7 ml. 2N HCl treated with 0.01 mole NaNO2 gave V, brown .apprx.240°, exploding at 250°. The ultraviolet spectral curves were given for a number of the above compds.

CC 10G (Organic Chemistry: Heterocyclic Compounds)

IT 1931-03-9P, 2(1H)-Pyrimidinone, 4,5-diamino-1-methyl-
6220-47-9P, Cytosine, N-methyl- 23899-73-2P, 2(1H)-Pyrimidinone
, 4,5-diamino- 23899-77-6P, 2(1H)-Pyrimidinone,
4,5-diamino-1-β-D-ribofuranosyl- 51141-43-6P, v-Triazolo[4,5-
d]pyrimidin-5(6H)-one 52093-83-1P, 9H-Purin-2(1H)-one, 9-methyl-
69100-00-1P, Cytosine, 1-methyl-5-nitro- 72346-25-9P, Purin-2(1H)-one,
1-β-D-ribofuranosyl- 78197-95-2P, Purin-2(1H)-one, 1-methyl-
88187-93-3P, 2(1H)-Pyrimidinone, 4,5-diamino-1-β-D-
ribofuranosyl-, hydrochloride 100347-87-3P, Purin-2(1H)-one,
1-β-D-glucopyranosyl- 102161-68-2P, Purin-2(1H)-one,
1-β-D-glucopyranosyl-, tetraacetate 104096-91-5P, 2(1H)-
Pyrimidinone, 5-amino-4-methylamino- 107626-04-0P, 2(1H)-
Pyrimidinone, 4,5-diamino-1-β-D-glucopyranosyl-, tetraacetate
110392-97-7P, Cytosine, 1-β-D-glucopyranosyl-5-nitro-, tetraacetate
114252-95-8P, Cytosine, 1-β-D-glucopyranosyl-5-nitro- 118661-14-6P,
v-Triazolo[4,5-d]pyrimidin-5(6H)-one, 6-β-D-ribofuranosyl-
120883-87-6P, Cytidine, 5-nitro- 122336-54-3P, Cytidine, 5-nitro-,
tribenzoate 127734-87-6P, Mercury, bis(4-amino-5-nitro-2-oxo-1(2H)-

pyrimidinyl)- 127734-87-6P, Cytosine, 1,1'-mercuribis[5-nitro-
RL: PREP (Preparation)
(preparation of)

L79 ANSWER 36 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1960:44680 ZCAPLUS Full-text
DOCUMENT NUMBER: 54:44680
ORIGINAL REFERENCE NO.: 54:8831a-h
TITLE: Pyrimidine nucleosides. V. 2-Oxohexahydropyrimidines and their nucleosides
AUTHOR(S): Fox, Jack J.; Praag, Dina Van
CORPORATE SOURCE: Cornell Univ., New York, NY
SOURCE: Journal of the American Chemical Society (1960), 82, 486-9
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
AB cf. C.A. 53, 7190f. The heterocyclic nucleus of 4-thiothymidine (I) and 4-thiouridine (II) is reduced unexpectedly by activated Raney Ni. 2-Hydroxypyrimidines are reduced over Rh-Al2O3 catalyst to the corresponding N,N'-trimethyleneureas while uracil and 1-methyluracil are reduced over Raney Ni or Rh-Al2O3 to the corresponding 5,6-dihydro derivs. 2-Ethoxy-4(3H)-pyrimidinone (7.0 g.) and 33 g. P2S5 refluxed 2 hrs. in pure C5H5N while 1.0 cc. H2O was being added slowly, about 50% of the C5H5N removed in vacuo, poured with stirring into H2O, filtered, concentrated to near dryness, dissolved in dilute NH4OH, treated with C, acidified, and cooled gave 3.2 g. 4-thiouracil (III), yellow prisms, m. 289-90° (decomposition) (hot H2O). MeNHCONH2 (3.7 g.) in 20 cc. EtOH and 10 cc. concentrated HCl treated with 11.0 g. tetraethoxypropane, stirred 1 hr. at 60°, cooled, and filtered, the residue washed with Et2O, dissolved in aqueous Na2CO3, adjusted to pH 5 with dilute H2SO4, and evaporated, and the residue extracted in a Soxhlet apparatus with 250 cc. Me2CO gave 4.0 g. 1,2-dihydro-1-methyl-2-pyrimidinone, m. 125-6°; picrate m. 162°. III (1 28 g.) in 400 cc. EtOH refluxed 15 min. with stirring with 6 g. activated Raney Ni gave 0.6 g. N,N'-trimethyleneurea (IV), m. 259-60° (hot EtOH). 2-Hydroxypyrimidine (V) (0.48 g.) in 200 cc. EtOH refluxed 15 min. with 4 g. activated Raney Ni yielded 450 mg. IV, m. 258-9°. V (0.96 g.) in 400 cc. H2O hydrogenated 0.5 hr. under ambient conditions over 0.9 g. Rh-Al2O3 gave 0.8 g. IV. CH2(CH2NH2)2 (7.4 g) and 71.4 (PhO)2CO heated 3 hrs. in a sealed tube at 180°, cooled, and diluted with 150 cc. EtOH yielded 4.8 g. IV. 1-Methyl-4-thiouracil (1.42 g.) and 6 g. Raney Ni in EtOH refluxed 15 min. yielded 0.8 g. N-Me derivative (VI) of IV, m. 86-9° (sublimed at 130°/1 mm.); picrate (VII) m. 134-5° (EtOH). The course of the desulfurization was followed spectrally by adding the Raney Ni gradually during 2 hrs. 1-Methyl-2-pyrimidinone (220 mg.) and 2 g. Raney Ni refluxed 15 min. in EtOH, filtered, and treated with picric acid gave 500 mg. VII, m. 134-5°. 1-Methyl-2-pyrimidinone hydrogenated in the usual manner over Rh-Al2O3 gave 80% VI, m. 86-9°. 1-(3,5-Di-O-benzoyl-2-deoxy-β-D-ribosyl)-4-thiothymine (4.66 g.) in 500 cc. EtOH refluxed 15 min. with stirring with 16 g. activated Raney Ni, filtered, and evaporated yielded 2.8 g. N-(3,5-di-O-benzoyl-2-deoxy-β-D-ribofuranosyl)-2-oxo-5- methylhexahydropyrimidine, m. 135-6°. I (770 mg.) in 200 cc. absolute EtOH refluxed 15 min. with 5 g. wet activated Raney Ni, filtered, and evaporated, and the residue dissolved in a small amount of EtOH and refrigerated several weeks yielded 0.2 g. N-(2-deoxy-β-D-ribofuranosyl)-2-oxo-5- methylhexahydropyrimidine, needles, m. 186-7°. 1-(2,3,5-Tri-O-benzoyl-β-D-ribosyl)-4-thiouracil (5.72 g.) reduced in the usual manner with Raney Ni gave 3.0 g. N-(2,3,5-tri-O-benzoyl-β-D- ribosyl)-2-oxohexahydropyrimidine, needles, m. 143-5°. Uracil (1.12 g.) in 500 cc. H2O refluxed 2 hrs. with 15 g. activated Raney Ni gave 560 mg. 5,6-dihydrouracil, m. 269-70°. 1-

Methyluracil (1.26 g.) in 400 cc. EtOH refluxed 6 hrs. with stirring with 20 g. Raney Ni gave 0.47 g. 4,5-dihydro derivative, m. 169-70°, also obtained in 86% yield by hydrogenation in H2O over Rh-Al2O3 at room temperature

CC 10G (Organic Chemistry: Heterocyclic Compounds)

IT 1852-17-1, 2(1H)-Pyrimidinone, tetrahydro-
(and derivs., and their nucleosides)

IT 591-28-6P, Uracil, 4-thio- 696-11-7P, Hydrouracil, 1-methyl- 3739-81-9P, 2(1H)-Pyrimidinone, 1-methyl- 10166-54-8P, 2(1H)-Pyrimidinone, tetrahydro-1-methyl- 52523-24-7P, 2(1H)-Pyrimidinone, 1-β-D-ribofuranosyl-, tribenzoate 92788-30-2P, 2(1H)-Pyrimidinone, tetrahydro-1-methyl-, picrate 96254-24-9P, 2(1H)-Pyrimidinone, 1-methyl-, picrate 106531-39-9P, 5H-Dipyrido[1,2-a:3',2'-e]pyrimidin-5-one 121970-08-9P, 2(1H)-Pyrimidinone, 1-(2-deoxy-β-D-ribofuranosyl)tetrahydro-5-methyl-, dibenzoate 122360-93-4P, 2(1H)-Pyrimidinone, 1-(2-deoxy-β-D-ribofuranosyl)tetrahydro-5-methyl-
RL: PREP (Preparation)
(preparation of)

L79 ANSWER 37 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1960:17044 ZCAPLUS Full-text
DOCUMENT NUMBER: 54:17044
ORIGINAL REFERENCE NO.: 54:3443c-h
TITLE: Simple syntheses of pyrimidine 2'-deoxyribonucleosides
AUTHOR(S): Hoffer, Max; Duschinsky, Robert; Fox, Jack J.; Yung, Naishun
CORPORATE SOURCE: Hoffmann-La Roche Inc., Nutley, NJ
SOURCE: Journal of the American Chemical Society (1959), 81, 4112-13
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 54:17044

AB cf. C.A. 52, 2866h, 565d. The total syntheses are reported of pyrimidine 2'-deoxyribonucleosides by the mercuri procedure (C.A. 53, 8145h). Crystalline 3,5-di-O-p-chloro(or p-methyl)-benzoyl-2-deoxy-D-ribosyl chlorides coupled readily with the relatively more reactive monomercurypirimidines to yield (after deacylation) α- and β-anomers of 2'-deoxynucleosides. (All m.ps. are uncor. M.ps. of mixts. of the α- and β-anomers were depressed.) Me 2-deoxy-D-ribofuranoside (I) yielded 75% 3,5-di-O-p-toluoyl derivative (II), m. 76.5°, [α]D -6.2° (CHCl3). II with AcOH-HCl gave 70% 3,5-di-O-p-toluoyl-2-deoxy-D-ribosyl chloride (III), m. 109°, [α]D 108° (HCONMe2). 2-Deoxy-D-ribose yielded 65% 3,5-di-O-p-chloro analog (IV) of I, m. 118-20°. 1-Acetylthymine refluxed with Hg(OAc)2 in MeOH yielded monomercurithymine (V). 5-Fluorouracil and Hg(OAc)2 in refluxing aqueous MeOH yielded monomercuri-5-fluorouracil (VI); similarly, 5-fluorocytosine yielded monomercuri-5-fluorocytosine (VII). III condensed with V in hot PhMe yielded 50% 3',5'-di-O-p-toluoylthymidine (VIII), m. 197°, [α]D -50° (pyridine). VIII on deacylation gave thymidine. The mother liquors yielded 4% α-isomer (IX) of VIII, m. 138°, [α]D -14.5° (pyridine). IX on deacylation yielded α-thymidine (X), m. 187°, [α]D 7.2° (H2O). Similarly, III with VI yielded anomers of 1(3',5'-di-O-p-toluoyl-2-deoxy-D- ribosyl)-5-fluorouracil (XI): α-XI (27% from mother liquors), m. 214-15°, [α]D -72.5° (pyridine); β-XI (41% top fraction from pyridine) m. 229°, [α]D -17° (pyridine). Deacylation of XI yielded α-5-fluoro-2'-deoxyuridine (α-XII), m. 150-1°, [α]D -21° (H2O), and β-XII, m. 150-1°, [α]D 37.5° (H2O). VII condensed with either III or IV and the product deacylated yielded a crystalline mixture, m. 167-70°, [α]D -0.7°, of 5-fluoro-2'-deoxycytidine (XIII) anomers,

which showed about 50% of the activity of authentic β-XIII. N-Acetylcytosine-mercury condensed with IV in hot xylene gave anomers of 1-(3',5'-di-O-p-chlorobenzoyl-2-deoxy-D-ribosyl)-4- acetamido-2(1H)-pyrimidinone (XIV): α-XVI (22% yield) m. 204.5-205°, [α]D -66° (CHCl3); β-XIV (32% yield) m. 128-30°, [α]D -19°. Deacylation of α-XIV and β-XIV gave high yields of cytosine 2'-deoxynucleosides (XV): α-XV, m. 192-3°, [α]D -44°; β-XV, m. 200-1°, [α]D 78° (N NaOH), m.p. of a mixture with 2'-deoxycytidine not depressed.

CC 10G (Organic Chemistry: Heterocyclic Compounds)

L79 ANSWER 38 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1960:110586 ZCAPLUS Full-text
DOCUMENT NUMBER: 54:110586
ORIGINAL REFERENCE NO.: 54:21114c-i,21115a-i,21116a
TITLE: Thiation of nucleosides. II. Synthesis of 5-methyl 2'-deoxycytidine and related pyrimidine nucleosides
AUTHOR(S): Fox, Jack J.; Van Praag, Dina; Wempen, Iris; Doerr, Iris L.; Cheong, Loretta; Knoll, Joseph E.; Eidinoff, Maxwell L.; Bendich, Aaron; Brown, George Bosworth
CORPORATE SOURCE: Sloan-Kettering Div. of Cornell Univ., New York, NY
SOURCE: Journal of the American Chemical Society (1959), 81, 178-87
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 54:110586

AB cf. CA 52, 13736i. Thiation of suitably blocked pyrimidine nucleosides was accomplished with P2S5 (I) in C5H5N (II). The resulting 4-thio derivs. were utilized as intermediates in the preparation of other 4-substituted pyrimidine nucleosides. 1-Methyluracil (12.6 g.), 6.6 g. I, and 400 ml. II, stirred and refluxed 3 hrs., concentrated to 250 ml. in vacuo, filtered, the filtrate concentrated to dryness and crystallized from alc. gave 1-methyl-4-thiouracil in 62% yield, m. 193-4° (H2O), λmaximum 244 and 333 mμ, λmin. 277 mμ (pH 7). This product (500 mg.) in 30 ml. alc. NH3, heated in a sealed tube 24 hrs. at 120°, precipitated 300 mg. 1-methylcytosine, establishing 4-thiation in 1-substituted pyrimidines. Thymidine (III) (0.083 mole) in 600 ml. II, treated 65 hrs. with 0.166 mole BzCl ((V) at 50-5°, the solution poured over ice with stirring until solidification, the solid filtered off, stirred 15 min. with ice H2O, filtered, pressed dry and recrystd. from boiling alc., gave 85% 1-(3,5-di-O-benzoyl-2-deoxy-β-D-ribofuranosyl)thymine (V), m. 192.5-3.5. Similarly, III (0.02 mole) and 0.06 mole IV in II gave 9.1 g. tribenzoylthymidine, m. 125-6° (alc.), and 0.33 mole uridine (VI) and 1.1 mole IV in II gave 167 g. 1-(2,3,5-tri-O-benzoyl-β-D- ribofuranosyl)uracil (VII), m. 142-3° (C6H6). VI treated with a large excess of IV 3 hrs. at room temperature, the product poured over ice, stirred 1 hr., the H2O decanted, the residue dissolved in CHCl3, washed with H2O, cold 2N H2SO4, NaHCO3 solution, and H2O, the solution dried, and the CHCl3 removed gave an oil which kept several days in alc.-Et2O precipitated tetrabenzoyluridine, m. 147-8°, mixed m.p. with VII 134-41°. VII (5.56 g.), 8.88 g. I and 150 ml. II, refluxed 5 hrs. with stirring, 50 ml. II removed, the remainder poured into H2O, the resulting oil dissolved in CHCl3, filtered, the filtrate washed with H2O, dried, concentrated to dryness in vacuo, the residue dissolved in hot alc. and cooled, gave 4.96 g. crystalline 1-(2,3,5-tri-O-benzoyl-β-D-ribofuranosyl)-4-thiouracil (VIII), m. 128-30° (alc.). In similar thiations, small amts. of H2O added to the reaction mixture to a permanent orange turbidity increased yields and made product isolation easier. Thus, 20 g. V, and 37 g. I in 600 ml. II treated dropwise with 1.8 ml. H2O, the orange, turbid mixture refluxed 4 hrs. and worked up as in the case of VIII gave 15 g. 1-(3,5-di-O-benzoyl- β-D-2-deoxyribofuranosyl)-4-thiothymine (IX), m. 159-60° (alc.), [α]25D -52° (c

1.2, CHCl3). Similarly prepared were 83% 1-(2,3,5-tri-O-benzoyl-β-D-ribofuranosyl)-4-thiothymine (X), m. 190-1° (alc.), and 87% 1-(2,3,5-tri-O-benzoyl-β-D- xylofuranosyl)-4-thiothymine (XI), m. 166-8°, from 1-(2,3,5-tri-O-benzoyl-β-D-ribofuranosyl)thymine and 1-(2,3,5-tri-O-benzoyl-β-D-xylofuranosyl)thymine, resp. IX (7.0 g.) treated 24 hrs. with 80 ml. alc. NH3 at 100° (sealed tube), the green solution concentrated, dissolved in H2O, the BzOEt distilled in vacuo, the aqueous solution extracted with CHCl3, treated with, C, filtered, concentrated to dryness, dissolved in warm alc. with addition of HCl precipitated 2.85 g. 1-(2-deoxy-β-D-ribofuranosyl)-5-methylcytosine-HCl (XII), m. 154-5° (decomposition), [α]23D 54° (c 1.02, N HCl), λmaximum 208 and 277 mμ, λmin. 255 mμ (pH 7); picrate, darkens at 170-230°. XII with NaNO2 in H2O at 60° gave III, m. 183-4°. XII with 72% HClO4 at 100° gave 5-methylcytosine. Treatment of VIII, X, and XI with alc. NH3 as in the preparation of XII gave the following (product, % yield, m.p., and recrystn. solvent given): cytidine (XIII) (as the sulfate), 89, 222-3°, alc.; 5-methyl-cytidine (XIV), 80, 210-11°, 90% alc.; 1-(β-D-xylofuranosyl)-5-methylcytosine (XV), 50, 205-7°, alc. [XV.HCl, m. 207-8° (aqueous alc.), [α]23D -2.5° (for the HCl salt, c 1.0, N NaOH)]. 1-(Tetra-O-acetyl-β-D-glucopyranosyl)thymine (4.0 g.), 7.4 g. I, 125 ml. II, and 0.3 ml. H2O refluxed 6 hrs. and worked up as in the preparation of IX gave 1.7 g. glass, which treated with NH3 as in the preparation of XII gave crystalline 1-(β-D-glucopyranosyl)-5-methylcytosine, m. 279-80° (90% alc.), [α]23D -4° (c 2.4, N NaOH). IX (9.32 g.) in 0.5 l. warm MeOH, treated dropwise with 25 ml. N NaOMe in MeOH, refluxed 4 hrs., made acidic (pH 5) with AcOH, concentrated to dryness, dissolved in H2O, extracted with CHCl3, the aqueous solution concentrated to dryness, extracted with Me2CO, and the Me2CO removed, gave 4.5 g. impure, glassy 4-thiothymidine (XVI). This product oxidized with I by the method of Miller (CA 40, 14556) gave thymidine disulfide (XVII), m. 200-3°, λmaximum 257 and 321 mμ, λmin. 238 and 282 mμ (pH 7.4). Similarly, 11.4 g. VIII yielded 3.9 g. 4-thiouridine (XVIII), λmaximum 244 and 328 mμ, λmin. 225 and 272 mμ (pH 7.4). XVIII oxidized with I gave uridine disulfide, m. 188-90°, λmaximum 261 and 309 mμ, λmin. 236 and 278 mμ (pH 7.4). Treatment of this compound with alc. NH3 as in the preparation of XIII from VIII gave XIII sulfate, m. 221-2°. Treatment of IX with alc. MeNH2 at 100° (sealed tube) gave 1-(2-deoxy-β-D-ribofuranosyl)-4-methylamino-5-methyl-2(1H)- pyrimidinone (XIX), m. 225-7°, [α]25D 28° (c 1.2, H2O), λmaximum 275 mμ and 235 mμ (shoulder), pKa 4.04. Similarly, VIII gave 1-(β-D-ribofuranosyl)-4-methylamino-2(1H)- pyrimidinone, m. 202-3° (alc.) λmaximum 237 mμ and 234 mμ (shoulder), λmin. 252 mμ (pH 7.4). VIII and IX with Ph(CH2)2NH2 gave 1-(β-D-ribofuranosyl)-4-(β-phenylethylamino)- 2(1H)-pyrimidinone, m. 205-6° (alc.), λmaximum 241 and 272.5 mμ, λmin. 229 and 247 mμ (pH 7), and 1-(2-deoxy-β-D-ribofuranosyl)-4-(β-phenylethylamino)-5-methyl-2(1H)-pyrimidinone (XX), m. 183-5° (Et2O-alc.), λmaximum 277.5 mμ, λmin. 252.5 mμ, shoulder at 240 mμ, pKa 3.83. NH2OH in MeOH refluxed 4 hrs. with IX gave 74% 1-(2-deoxy-3,5-di-O-benzoyl-β-D-ribofuranosyl)- 4-hydroxylamino-5-methyl-2(1H)-pyrimidinone, m. 169-70°, on removal of solvent and recrystn. from alc. XVI (1 g.) in alc., refluxed 4 hrs. with 6.5 g. NH2OH, gave 0.1 g. 1-(2-deoxy-β-D-ribofuranosyl)-4- hydroxylamino-5-methyl-2(1H)-pyrimidinone hemihydrate (XXI), m. 114° (MeOH), pKa 2.3 and 11.1. Similarly, XVIII (520 mg.) and NH2OH gave 250 mg. 1-(β-D-ribofuranosyl)-4-hydroxylamino-2(1H) pyrimidinone (XXII), m. 169-72° (MeOH), λmaximum 236 and 272 mμ, λmin. 262 mμ (pH 7), pKa 2.26 and 10.5. IX (8.0 g.) in 600 ml. alc., refluxed 1 hr. with 28 ml. (NH2)2, concentrated in vacuo, the BzOEt removed by codistn. with H2O, the residue crystallized from alc., gave 3.1 g. 1-(2-deoxy-β-D-ribofuranosyl)-4-hydrazino-5-methyl-2(1H)-

pyrimidinone (XXIII), m. 178-9°, [α]25D 30°, λmaximum 277.5 mμ, λmin. 252.5 mμ (pH 7). This compound was also prepared by treating XVI or XVII with N2H4. XXIII (3.0 g.) in dilute AcOH, cooled, treated with 3.3 g. NaNO2 in 50 ml. H2O, concentrated in vacuo, the residue triturated with alc., filtered, the filtrate concentrated, gave a substance, C10H13N5O (XXIV), m. 148-9°, possibly 5,6-dihydro-6-(2-deoxy-β-D-ribofuranosyl)-8-methyl-5-tetrazolo [c] pyrimidinone. 4-Ethoxy-2(1H)-pyrimidinone (14 g.) in 0.5 l. alc. refluxed 2 hrs. with 50 ml. N2H4, the solvent removed in vacuo and the residue crystallized from 95% alc. gave 12 g. 4-hydrazino-2(1H)-pyrimidinone, m. 305-10° (decomposition), λmaximum (pH 7) 268 mμ, λmin. 247 mμ. This compound (1.26 g.) in dilute AcOH cooled and treated with 2.8 g. NaNO2 gave 0.89 g. of a substance, C4H3N5O, m. 241-2° (decomposition), possibly 5(1H)-tetrazolo [c] pyrimidinone analogous to XXIV. 1,5-Dimethyl-4-ethoxy-2(1H)-pyrimidinone (0.4 g.) treated at 150° (sealed tube) with 30 ml. NH3 in alc., the solvent removed and the residue crystallized from alc. gave 250 mg. 1,5-dimethylcytosine, m. 308-9°, λmaximum 280 mμ, λmin. 253 mμ (pH 7), pKa 4.76. The ultraviolet spectra of compds. XII, XIV-XVI, and XIX-XXIV were determined at various pH values and spectrophotometrically calculated pKa values were compared. Substitution on the 1- or 5-position of the pyrimidine ring raised the pKa for basic dissociation.

CC 10G (Organic Chemistry: Heterocyclic Compounds)

IT 554-01-8P, Cytosine, 5-methyl- 838-07-3P, Cytidine, 2'-deoxy-5-methyl- 1122-47-0P, Cytosine, 1-methyl- 1748-04-5P, Uridine, 2',3',5'-tribenzoate 1867-17-0P, Cytidine, 2'-deoxy-N-hydroxy-5-methyl- 2140-61-6P, Cytidine, 5-methyl- 3258-02-4P, Cytidine, N-hydroxy- 3310-41-6P, 2(1H)-Pyrimidinone, 4-hydrazino- 6018-48-0P, Cytidine, sulfate 10578-79-7P, Cytidine, N-methyl- 13957-31-8P, Uridine, 4-thio- 15049-50-0P, Uridine, 4-thio-, 2',3',5'-tribenzoate 17634-60-5P, Cytosine, 1,5-dimethyl- 18265-48-0P, Cytosine, 1-β-D-glucopyranosyl-5-methyl- 18312-90-8P, 2(1H)-Pyrimidinone, 1-(2-deoxy-β-D-ribofuranosyl)-4-hydrazino-5-methyl- 18427-02-6P, 2(1H)-Pyrimidinone, 4,4'-dithiobis[1-β-D-ribofuranosyl- 18492-10-9P, Cytosine, 5-methyl-1-β-D-xylofuranosyl- 21028-18-2P, Cytosine, 5-methyl-1-β-D-xylofuranosyl-, hydrochloride 25406-44-4P, Cytidine, 2'-deoxy-N,5-dimethyl- 28585-48-0P, Uridine, 5-methyl-4-thio-, 2',3',5'-tribenzoate 34948-48-6P, Cytidine, 2'-deoxy-5-methyl-N-phenethyl- 35455-86-8P, Uracil, 1-methyl-4-thio- 35898-30-7P, Thymidine, 3',5'-dibenzoate 68027-42-9P, Thymine, 4-thio-1-β-D-xylofuranosyl-, 2',3',5'-tribenzoate 68696-19-5P, Cytidine, 2'-deoxy-5-methyl-, hydrochloride 103388-15-4P, 2(1H)-Pyrimidinone, 4,4'-dithiobis[5-methyl-1-β-D-ribofuranosyl- 109721-75-7P, Cytidine, N-phenethyl-, hydrochloride 117862-70-1P, Cytidine, N,5-dimethyl- 119482-37-0P, Uridine, 3-benzoyl-, 2',3',5'-tribenzoate 123103-76-4P, Cytidine, 2'-deoxy-N-hydroxy-5-methyl-, 3',5'-dibenzoate 124130-15-0P, Thymidine, 3-benzoyl-, 3',5'-dibenzoate
RL: PREP (Preparation)
(preparation of)

L79 ANSWER 39 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1958:15815 ZCAPLUS Full-text
DOCUMENT NUMBER: 52:15815
ORIGINAL REFERENCE NO.: 52:2866h-i,2867a-i,2868a
TITLE: Pyrimidine nucleosides. III. Synthesis of cytidine and related pyrimidine nucleosides
AUTHOR(S): Fox, Jack J.; Yung, Naishun; Wempen, Iris; Doerr, Iris L.
CORPORATE SOURCE: Cornell Univ. Med. Coll., New York, NY

SOURCE: Journal of the American Chemical Society (1957), 79, 5060-4
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable
OTHER SOURCE(S): CASREACT 52:15815

AB cf. C.A. 51, 14743a. Acetylcytosine (I) (3.06 g.) in 1500 cc. H2O treated with 20 cc. N NaOH, warmed with stirring below 50° until dissolved, filtered, treated with stirring with 5.43 g. HgCl2 in EtOH, warmed to about 70°, cooled to 40°, treated with 0.02 mole NaOH, warmed again to 70°, cooled, and filtered, and the residue washed and dried gave 6.9 g. N-acetylcytosinemercury (II). II gave with concentrated alkali HgO. 4-Ethoxy-2(1H)-pyrimidinone (0.05 mole) (III) in 500 cc. H2O containing 0.05 mole NaOH treated with stirring with 0.05 mole HgCl2 in EtOH yielded 17.8 g. chloromercuri derivative (IV) of III. II (2.0 g.) and 150 cc. PhMe dried azeotropically by distillation of about 1/4 of the solvent, the hot mixture treated with stirring with 2.3 g. acetobromoglucose (V), refluxed a few min., treated with an addnl. 0.0057 mole V, refluxed again, cooled, diluted with 500 cc. petr. ether, cooled, and filtered, the residue dissolved in CHCl3, the insol. portion (0.25 g.) discarded, the filtrate washed with 30% aqueous KI and H2O, dried, and evaporated in vacuo, and the residual sirup dissolved in the min. amount hot EtOH and refrigerated 2 days gave 2.2 g 1-(tetra-O-acetyl-β-D-glucopyranosyl)-4-acetamido-2(1H)- pyrimidinone, m. 217-18° (EtOH). 1-O-acetyl-2,3,5-tri-O-benzoyl- D-ribose (VI) (0.01 mole) and 150 cc. dry Et2O previously saturated at 0° with HCl kept 4 days at 5-10°, the solvent evaporated in vacuo, the sirupy residue evaporated 3 times in vacuo with 50 cc. dry C6H6 each, dissolved in C6H6 and added to 0.005 mole II in dry hot xylene, the mixture refluxed 25 min., cooled, diluted with petr. ether, and filtered, the residue dissolved in CHCl3, the solution washed with 30% aqueous KI and H2O, dried, and evaporated, and the residual sirup dissolved in the min. amount hot EtOAc, diluted with petr. ether to incipient cloudiness, and cooled yielded 1.5 g. 1-(tri-O-benzoyl-β-ribofur.ovrhdot.anosyl)-4-acetamido-2(1H)- pyrimidinone (VII), m. 191-2° (corrected), [α]25589 -58°, [α]25546 -67°. Crude VII (3 g.) in 60 cc. EtOH previously saturated at 0° with NH3 heated in a sealed tube at 100° overnight, concentrated in vacuo, diluted with H2O, and distilled in vacuo to remove the EtOBz, the residue dissolved in H2O and washed with CHCl3, the aqueous solution treated with C and evaporated, the residue dissolved in a min. of hot 95% EtOH, and the hot solution treated with 4 drops concentrated H2SO4 and diluted to incipient turbidity with absolute EtOH yielded 1.07 g. cytidine (VIII).H2SO4, m. 224-5° with effervescence. 1-O-Acetyl-2,3,5-tri-O-benzoyl- α-D-xylose (5.0 g.) in 200 cc. dry Et2O saturated at 0° with dry HCl, kept 4 days at 5°, and concentrated in vacuo, the residual yellow sirup codistd. several times with C6H6 in vacuo, dissolved in C6H6, added with stirring to 1.75 g. II in dry hot xylene, refluxed 25 min., cooled, diluted with petr. ether, and filtered, the amorphous residue dissolved in CHCl3, the solution washed with 30% aqueous KI and H2O, dried and evaporated, and the residue dissolved in 1-2 cc. hot EtOAc, diluted with EtOH to incipient turbidity, and cooled gave 2.0 g. 1-(tri-O-benzoyl-β-D-xylofuranosyl)- 4-acetamido-2(1H)-pyrimidinone (IX), needles, m. 172-3° (corrected) (EtOAc-EtOH). Tetra-O-benzoyl-α-D-xylofuranose (5.6 g.) in 100 cc. dry CH2Cl2 saturated at 0° with dry HBr, kept 30 hrs. at room temperature, and poured with vigorous stirring in a thin stream into ice H2O, the organic layer washed rapidly with ice cold aqueous NaHCO3, dried, and evaporated, the residue dried azeotropically with C6H6 and dissolved in C6H6, the solution added to 0.005 mole II in dry hot PhMe, and the mixture worked up in the usual manner yielded 0.7 g. IX, m. 163-5° (uncor.). IX (0.70 g.) heated overnight at 100° in a sealed tube with 30 cc. MeOH previously saturated with NH3 at O°, and the mixture worked up as for VIII gave 220 mg. 1-β-D-xylofuranosylcytosine (X), m.

237-8°. X consumed in 2 days 1 mole NaIO4 without the liberation of HCO2H; the resulting dialdehyde solution showed [α]25D 38° (c 0.7, H2O). VIII gave similarly a dialdehyde solution, [α]25D 39°. IV (3.75 g.) in 200 cc. dry hot xylene treated with 4.1 g. V, refluxed 40 min. with stirring, cooled, treated with 1 l. petr. ether, and filtered, the residue dissolved in CHCl3, the solution filtered, washed with aqueous KI, dried, and evaporated, and the residual sirup triturated with EtOHEt2O yielded 1.1 g. crystalline 1-(tetra-O-acetyl-β-D-glucopyranosyl)-4-ethoxy-2(1H)- pyrimidinone (XI), m. 203-4° (EtOH). XI and HCl in MeOH gave 1-β-D-glucopyranosyluracil, m. 199-201°. VI (0.02 mole) and 250 cc. dry Et2O previously saturated with HCl at 0° kept 4 days at 5-10° and evaporated in vacuo, the residue dried azeotropically in the usual manner and dissolved in C6H6, the solution added to 7.5 g. IV in dry hot xylene, the mixture refluxed 25 min. with stirring, cooled, treated with petr. ether, and filtered, the residue dissolved in CHCl3, the solution worked up in the usual manner, and the residual sirup dissolved in the min. volume warm EtOAc, diluted with Et2O, and cooled overnight yielded 0.3 g. VI; the filtrate yielded 3.7 g. ribofuranosyl analog (XII) of XI, powder, m. 96-106°; the mother liquor from the XII gave 3.2 g. lower melting material. Crude XII (1.5 g.) heated in a sealed tube overnight at 100° with 50 cc. alc. NH3 and worked up in the usual manner gave 520 mg. VIII.H2SO4, m. 222-3° (aqueous EtOH). XII (0.4 g.) in 50 cc. EtOH treated with 2 cc. N NaOEt, refluxed 1 hr., acidified with 0.5 cc. concentrated HCl, filtered, refluxed 10 min., and concentrated, the sirupy residue dissolved in H2O and extracted with Et2O, and the aqueous solution treated with C, filtered, and analyzed spectrophotometrically showed the presence of uridine.

CC 10 (Organic Chemistry)

IT 50-99-7, D-Glucose 58-86-6, Xylose 7540-64-9, Ribose, D-, 5-phosphate 1-pyrophosphate
(2(1H)-pyrimidinone derivs.)

IT 3180-75-4P, Cytosine, N-acetyl-1-β-D-glucopyranosyl-, tetraacetate 3180-77-6P, Uracil, 1-β-D-glucopyranosyl- 3530-56-1P, Cytosine, 1-β-D-xylofuranosyl- 6018-48-0P, Cytidine, sulfate 7306-83-4P, 2(1H)-Pyrimidinone, 4-ethoxy-1-β-D-ribofuranosyl-, tribenzoate 14631-20-0P, Cytosine, N-acetyl-, mercury derivative 23707-29-1P, 2(1H)-Pyrimidinone, 4-ethoxy-1-β-D-glucopyranosyl-, tetraacetate 27391-03-3P, Cytidine, N-acetyl-, tribenzoate 92457-90-4P, 2(1H)-Pyrimidinone, 1-(chloromercuri)-4-ethoxy- 92457-90-4P, Mercury, (4-ethoxy-2-oxo-1(2H)-pyrimidinyl)-, chloride 119439-00-8P, Cytosine, N-acetyl-1-β-D-xylofuranosyl-, tribenzoate
RL: PREP (Preparation)
(preparation of)

L79 ANSWER 40 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1954:7622 ZCAPLUS Full-text
DOCUMENT NUMBER: 48:7622
ORIGINAL REFERENCE NO.: 48:1458i,1459a-c
TITLE: The identification of cytidylic acids a and b by spectrophotometric methods
AUTHOR(S): Fox, Jack J.; Cavalieri, Liebe F.; Chang, Naishun
CORPORATE SOURCE: Sloan-Kettering Inst. for Cancer Research, New York, NY
SOURCE: Journal of the American Chemical Society (1953), 75, 4315-17
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. C.A. 47, 8131c. The study of the variations in the UV spectra of several pyrimidine nucleosides in the high alkaline range has been continued. These spectral variations which occur at pH 12-14 are caused by the ionization of the 2'-OH group of the sugar, with a limited contribution from the other OH groups. On this basis it has been possible to confirm the identity of cytidylic acids a (Ia) and b (Ib) as cytidine-2'-phosphate and the 3'-isomer, resp. Since uridylic acid b (IIb) may be obtained by the alkaline deamination of Ib, it is also concluded that uridylic acid a (IIa) and IIb are the 2'- and 3'-phosphates of uridine, resp. A mechanism whereby the ionization of the sugar moiety affects the chromophore of the pyrimidine ring is suggested. 1,3,4,6-Tetraacetyl-α-2-deoxy-D- glucose treated 2 days at 5° with HCl in Et2O, the solvent removed in vacuo, the residual sirupy 1-chloro-2-deoxy-3,4,6-triacetyl-D-glucose (3 g.) treated immediately with 3 cc. 2,4-diethoxy-pyrimidine, the mixture heated 48 h. at 95-100°, cooled, diluted with 10 cc. Et2O, and filtered from uracil, the filtrate let stand, the precipitate taken up in CHCl3, treated with Norite, and filtered, the filtrate evaporated to dryness, and the residue taken up in a min. of hot EtOH and cooled to 0° gave 0.4 g. 1-D-(2-deoxy-3,4,6-triacetylglucopyranosyl)-4-ethoxy-2-pyrimidone, m. 136-8° (from EtOH), which on hydrolysis with HCl in MeOH gave 1-D-2'-deoxyglucopyranosyluracil (III), m. 168-9° (from MeOH-Et2O). The spectrophotometrically determined apparent dissociation consts. for the 4-ammonium group of the following compds. are: cytidine (IV), 4.11; cytosine-2'-deoxyriboside, 4.25; Ib, 4.16; Ia, 4.30; cytosine-2'- deoxyriboside-5'-phosphate (V), 4.44. The UV spectra of Ia, Ib, III, IV, V, glucopyranosyluracil, 2'-deoxyribofuranosylcytosine, and 2',3'-isopropylideneuridine, m. 159-60°, are recorded.

CC 11B (Biological Chemistry: Methods and Apparatus)

IT 5139-56-0P, Uracil, 1-(2-deoxy-D-glucopyranosyl)- 5139-56-0P, Glucopyranoside, uracil-1 2-deoxy- 848942-31-4P, 2(1H)-Pyrimidinone, 1-(2-deoxy-D-glucopyranosyl)-4-ethoxy-, triacetate
RL: PREP (Preparation)
(preparation of)

L79 ANSWER 41 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1953:54086 ZCAPLUS Full-text
DOCUMENT NUMBER: 47:54086
ORIGINAL REFERENCE NO.: 47:9148b-e
TITLE: Absorption spectra and structure of 2-thiouracil derivatives as a function of pH
AUTHOR(S): Shugar, David; Fox, Jack J.
CORPORATE SOURCE: Free Univ. Brussels
SOURCE: Bulletin des Societes Chimiques Belges (1952), 61, 293-309
CODEN: BSCBAG; ISSN: 0037-9646
DOCUMENT TYPE: Journal
LANGUAGE: English

AB cf. C.A. 47, 3118g. Ultraviolet absorption spectra between 2000 and 3500 A. are given at pH values between 0 and 13 for 2-thiouracil pK1 7.75, pK2 12.7, its 6-Me (II) pK1 8.1, 1-Et (III) pK 8.7, and 3-Et (IV) 8.65 derivs., 2-methylthio-6-methyluracil (V) 7.9, 2-ethylthio-3-methyl-4(3H)- pyrimidone (VI) 0.9, 2-methylthio-3,6-dimethyl-4(3H)-pyrimidone (VII) 0.9, 1,3-diethyl-2-thiouracil (VIII), 2-ethylthio-1-methyl-4(1H)-pyrimidone (IX), and 2-ethylthio-4-ethoxy-6-methylpyrimidine (X). The apparent dissociation consts. (pK) were calculated from the differences in optical d. at a given wave length and the isosbestic points. I shows 2 sets of 3 isosbestic points indicating 2 equilibrium and II is similar although only pK1 was determined III, IV, V, VI, VII each show one set of 2 or 3 isosbestic points. Since the spectra of I, III, and IV in acid or near-neutral solns. are similar to that of VIII, they must all exist in the diketonic form at low pH values, and since the

curves of the first equilibrium of I are similar to those of IV, this equilibrium must involve the 1,2 tautomerism, and the 2nd equilibrium 3,4 tautomerism, that is, the 2 equilibrium refer to tautomerism and concomitant dissociation at the 2- and 4-positions, resp. The same holds for II. Comparison with the spectrum of IX suggests a quinoidal structure for III. The spectrum of V shows one equilibrium in alkaline solution similar to the 2nd and dissociation of I and II, and resembles that of X and not that of XII, suggesting that neutral and anionic V is probably dienolic. A comparison of the degrees of dissociation of I and II at blood pH places in question the necessity of assuming appreciable dissociation of these compds. for iodine absorption in antithyroid activity.

CC 3 (Electronic Phenomena and Spectra)

IT 1194-67-8, 4(3H)-Pyrimidinone, 3-ethyl-2-mercapto- 1195-10-4, Uracil, 1-ethyl-2-thio- 1198-19-2, Uracil, 1,3-diethyl-2-thio- 6328-58-1, 4-Pyrimidinol, 6-methyl-2-(methylthio)- 6328-58-1, 4(3H)-Pyrimidinone, 6-methyl-2-(methylthio)- 65592-65-6, 4(1H)-Pyrimidinone, 2-(ethylthio)-1-methyl- 99513-67-4, Pyrimidine, 4-ethoxy-2-(ethylthio)-6-methyl-
(spectrum of, effect of pH on)

IT 56-04-2, Uracil, 6-methyl-2-thio- 3240-60-6, 4(3H)-Pyrimidinone, 3,6-dimethyl-2-(methylthio)-
(spectrum of, pH and)

L79 ANSWER 42 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1953:46898 ZCAPLUS Full-text

DOCUMENT NUMBER: 47:46898

ORIGINAL REFERENCE NO.: 47:7895d-h

TITLE: Spectrophotometric studies of nucleic acid derivatives and related compounds as a function of pH

AUTHOR(S): Shugar, David; Fox, Jack J.

CORPORATE SOURCE: Univ. libre, Brussels, Belg.

SOURCE: Biochem. et Biophys. Acta (1952), 9, 199-218

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB The ultraviolet absorption spectra of a number of pyrimidines and related compds. were investigated over a wide enough pH range to show spectrophotometrically the limiting ionic species in each case and to permit calculation of the pK of the compound All measurements were made with a Beckman Model DU spectrophotometer using 10 mm. quartz cells. The compds. investigated and the spectrophotometrically determined apparent dissociation constants (pK) are given: cytosine, 4.45, 12.2; 5-methylcytosine, 4.6, 12.4; uracil, 9.5, 13; thymine, 9.9, > 13; 1-methyluracil, 9.75; 3-methyluracil, 9.95; 1,3-dimethyluracil (none); 2-ethoxy-4-hydroxypyrimidine, 8.2; 4-ethoxypyrimidone 10.7; 5-nitrouracil 5.3, 11.7; orotic acid .apprx.2.8, 9.45, >13; 2-methoxy-4-aminopyrimidine 5.3. These values agree well with previously published results. The variation of the spectra of these compds. with pH is shown in all cases to be explicable on the basis of ionic dissociation. Two ionic equilibria are shown in alkaline solution for uracil and thymine and the order of dissociation is shown to proceed through the 2- and 4-hydroxyl groups thus: Their structure is shown to be in the diketo form in neutral solution Cytosine and 5-methylcytosine in solns. up to pH 10 have structures represented by the lactam formula. The structure and spectra of other pyrimidine derivatives are discussed.

CC 3 (Electronic Phenomena and Spectra)

IT 2(1H)-Pyrimidinone, 4(or 6)-ethoxy-
4(?H)-Pyrimidinone, 2-ethoxy-
4(?H)-Pyrimidinone, 2-methoxy-6-methyl-
4(?H)-Pyrimidinone, 6-methyl-2-(methylthio)-
(spectrum of, pH and)

IT 56-04-2, Uracil, 6-methyl-2-thio- 65-71-4, Thymine 65-86-1, Orotic acid 66-22-8, Uracil 554-01-8, Cytosine, 5-methyl- 611-08-5, Uracil, 5-nitro- 874-14-6, Uracil, 1,3-dimethyl- 3240-60-6, 4(3H)-Pyrimidinone, 3,6-dimethyl-2-(methylthio)- 3289-47-2, Pyrimidine, 4-amino-2-methoxy- 6220-46-8, 2(1H)-Pyrimidinone, 4-ethoxy-1-methyl- 20461-60-3, Pyrimidine, 2,4-diethoxy- 25957-58-8, 4-Pyrimidinol, 2-ethoxy- 55996-28-6, 4-Pyrimidinol, 2-methoxy-6-methyl- (spectrum of, pH and)

L79 ANSWER 43 OF 43 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1952:20572 ZCAPLUS Full-text
DOCUMENT NUMBER: 46:20572
ORIGINAL REFERENCE NO.: 46:3540g-i,3541a-b
TITLE: The synthesis of nucleosides of cytosine and 5-methylcytosine
AUTHOR(S): Fox, Jack J.; Goodman, Irving
CORPORATE SOURCE: Univ. of Colorado, Boulder
SOURCE: Journal of the American Chemical Society (1951), 73, 3256-8
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. C.A. 42, 6326b. HCl (50 g.) passed during 40 min. into 20 g. β-D-glucose pentaacetate in 250 cc. Et2O at 5°, and the mixture refrigerated 2 days and concentrated in vacuo yielded 12.5 g. tetraacetyl-β-D-glucopyranosyl chloride (I), m. 98-9° (from anhydrous Et2O), [α]D26 -12°. Acetochloroxylose (II) (22 g.) and 22 g. 2,4-diethoxy-5-methylpyrimidine (IIA) heated (oven) 30 min. at 85°, 24 hrs. at 100°, and 24 hrs. at 110-15°, and the mixture cooled to room temperature and stirred with 1 volume Et2O yielded 14.3 g. 1,2-dihydro-2-oxo-4-ethoxy-5-methyl-1-(triacetyl-D- xylopyranosyl)pyrimidine (III), m. 189-90° (uncor.) (from EtOH). Acetobromoxylose (IV) yielded 34% III. For other halogenoses, the yields (%) from 2,4-diethoxypyrimidine and IIA are: D-acetobromo-glucose, 49, -; I, 65, -; D-acetobromogalactose, 37, -; D-acetochlorogalactose, 54, -; D- and L-acetobromoarabinose, 38, 43; D- and L-acetochloroarabinose, 58, 49; II, 31, 36; IV, 54, 48. 1,2-Dihydro-2-oxo-4-ethoxy-5-methyl-1-(D- xylopyranosyl)pyrimidine (4 g.) with HCl-MeOH (Hilbert, C.A. 31, 1771.7) yielded 2.2 g. 1-D-xylopyranosylthymine, m. 284-5° (decomposition) (from 1:1 alc.-water). 1-D-Glycopyranosylcytosines were prepared at 90° by the method of Hilbert and Jansen (C.A. 30, 1746.4). The compound, m.p. (uncor., dependent on rate of heating, decomposition), [α]D26 (water) are: xylosylcytosine, 251-2°, 24° (HCl salt, 225-30°, 21°; HNO3 salt, 223-7°, -); triacetyl-D-xylosyl-4-acetamidouracil, 277-8°, -; D-arabinosylcytosine, 265-7°, - 101° (HNO3 salt, 223-5°,-); L-arabinosylcytosine, 265-7°, 100°; glucosylcytosine-HCl, 200-1°, 20°; galactosylcytosine- HCl.H2O, 115-20° (effervescence), 48°; galactosylcytosine- HNO3, 140-1° (effervescence), 49°; xylosyl-5-methylcytosine, 254-6°, 14° [HCl salt, 246-7°,-; HNO3 salt, 231-2° (effervescence), -]; D-arabinosyl-5-methylcytosine, 290-1°, -79° [HNO3 salt, 206-10° (effervescence),-]; L-arabinosyl-5-methylcytosine, 290-1°, 78°.

CC 10 (Organic Chemistry)

IT 2(1H)-Pyrimidinone, 4-acetamido-1-D-xylosyl-, triacetate
Cytosine, D-arabinosyl-5-methyl-
Cytosine, D-arabinosyl-5-methyl-, nitrate
Cytosine, L-arabinosyl-
Cytosine, L-arabinosyl-5-methyl-
Glucoside, cytosine, hydrochloride
Uracil, triacetylxylosyl-4-acetylamino-
Xyloside, 4-acetamidouracil-1, triactate
RL: PREP (Preparation)

IT 4451-36-9P, Glucopyranosyl chloride, β-D-, tetraacetate 5040-16-4P, Cytosine, glucosyl-, hydrochloride 20197-24-4P, 2(1H)-Pyrimidinone, 4-ethoxy-5-methyl-1-D-xylopyranosyl-, triacetate 20566-05-6P, Cytosine, D-arabinosyl- 60993-53-5P, Cytosine, D-arabinosyl-, nitrate 95464-08-7P, Thymine, 1-D-xylopyranosyl-
RL: PREP (Preparation)
(preparation of)

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DICTIONARY FILE UPDATES:   2 AUG 2008  HIGHEST RN 1037774-47-2

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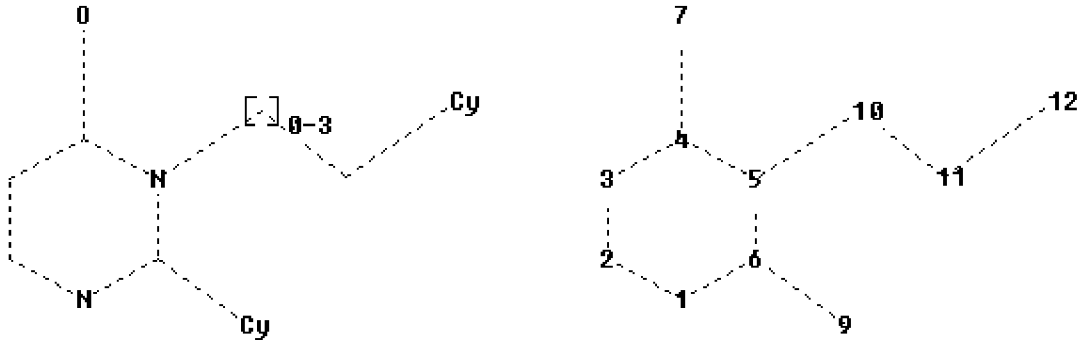


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ring nodes :
1  2  3  4  5  6
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ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6
exact/norm bonds :
1-2  1-6  2-3  3-4  4-5  4-7  5-6  5-10  6-9  10-11  11-12


Connectivity :
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Match level :
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Generic attributes :
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12:
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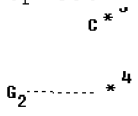
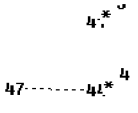
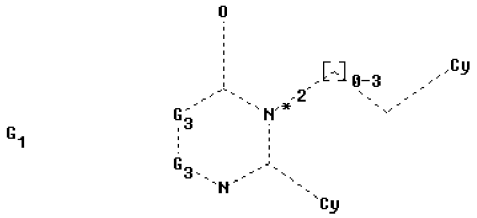
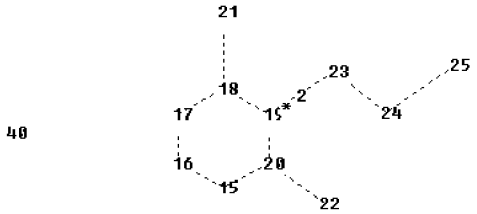
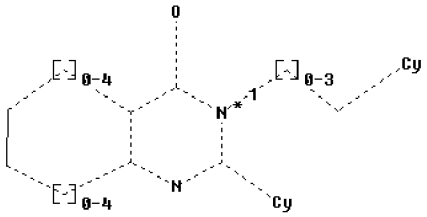
Uploading L6.str

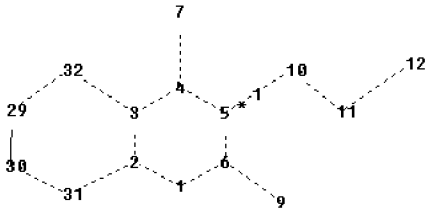












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ring bonds :
1-2 1-6 2-3 2-31 3-4 3-32 4-5 5-6 15-16 15-20 16-17 17-18 18-19 19-20
29-30 29-32 30-31
exact/norm bonds :
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20
16-17 17-18 18-19 18-21 19-20 19-23 20-22 23-24 24-25 29-32 30-31 44-47
exact bonds :
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isolated ring systems :
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G1:[*1],[*2]

G2:X,Cy,Ak

G3:[*3],[*4]

Connectivity :
4:3 E exact RC ring/chain 6:3 E exact RC ring/chain 7:1 E exact RC ring/chain
18:3 E exact RC ring/chain 20:3 E exact RC ring/chain 21:1 E exact RC ring/chain
41:2 E exact RC
ring/chain
Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:Atom 10:CLASS 11:CLASS
12:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS 22:Atom
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FILE LAST UPDATED: 3 Aug 2008 (20080803/ED)

ZCAplus now includes complete International Patent Classification (IPC)
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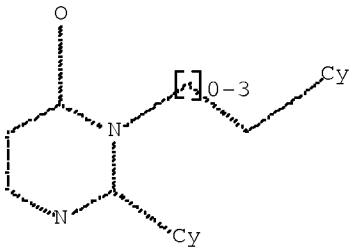
=> d stat que L9
L1   STR



Structure attributes must be viewed using STN Express query preparation.
L3 3630 SEA FILE=REGISTRY SSS FUL L1
L6 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L8 644 SEA FILE=REGISTRY SUB=L3 SSS FUL L6
L9 15 SEA FILE=ZCAPLUS ABB=ON PLU=ON L8

=> file casreact
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FILE CONTENT:1840 - 3 Aug 2008 VOL 149 ISS 6

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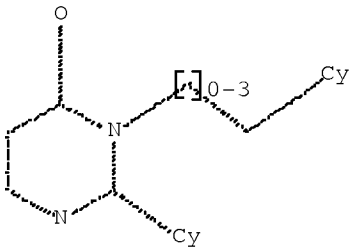
=> d stat que L11
L1 STR



Structure attributes must be viewed using STN Express query preparation.
L3 3630 SEA FILE=REGISTRY SSS FUL L1
L6 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L8 644 SEA FILE=REGISTRY SUB=L3 SSS FUL L6
L11 5 SEA FILE=CASREACT ABB=ON PLU=ON L8

=> file toxcenter
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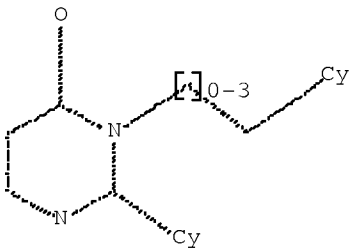
The BIOSIS segment of TOXCENTER has been augmented with 13,000 records from 1946 through 1968.

=> d stat que L13
L1 STR



Structure attributes must be viewed using STN Express query preparation.
L3 3630 SEA FILE=REGISTRY SSS FUL L1
L6 STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
L8 644 SEA FILE=REGISTRY SUB=L3 SSS FUL L6
L12 26 SEA FILE=REGISTRY ABB=ON PLU=ON L8 AND TOXCENTER/LC
L13 1 SEA FILE=TOXCENTER ABB=ON PLU=ON L12

=> file prousddr
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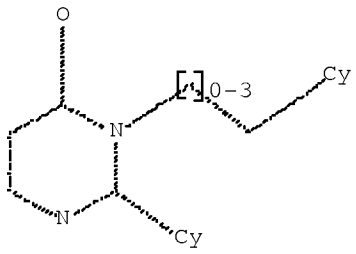
FILE COVERS 1980 TO 1 Jul 2008 (20080701/ED)

=> d stat que L17
L1 STR



Structure attributes must be viewed using STN Express query preparation.
L3 3630 SEA FILE=REGISTRY SSS FUL L1
L6 STR

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L8 644 SEA FILE=REGISTRY SUB=L3 SSS FUL L6
L15 1 SEA FILE=REGISTRY ABB=ON PLU=ON L8 AND P?/LC
L17 1 SEA FILE=PROUSDDR ABB=ON PLU=ON L15

=> file synthline
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FILE COVERS 1984 TO 16 Jun 2008 (20080616/ED)

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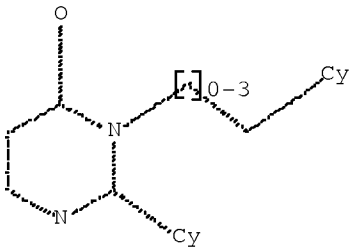
L1 STR

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Structure attributes must be viewed using STN Express query preparation.
L3         3630 SEA FILE=REGISTRY SSS FUL L1
L6              STR

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L8           644 SEA FILE=REGISTRY SUB=L3 SSS FUL L6
L16            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  L8 AND SY?/LC
L18            1 SEA FILE=SYNTHLINE ABB=ON  PLU=ON  L16


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FILE COVERS 1771 TO 2008.
*** FILE CONTAINS 10.322,808  SUBSTANCES ***

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   separate documents and can not be searched together in one query.
   Reaction data for BEILSTEIN compounds may be displayed
   immediately with the display codes PRE (preparations) and REA
   (reactions).  A substance answer set retrieved after the search
   for a chemical name, a compounds with available reaction
   information by combining with PRE/FA, REA/FA or more generally
   with RX/FA. The BEILSTEIN Registry Number (BRN) is the link
   between a BEILSTEIN compound and belonging reactions. For mo
   detailed reaction searches BRNs can be searched as reaction
   partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

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>>> Price change as of January 1st, 2008: Connect Time and Structure
    Search fees re-introduced. See NEWS and HELP COST <<<
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L1              STR
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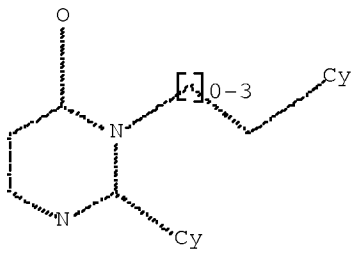


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Structure attributes must be viewed using STN Express query preparation.
L3         3630 SEA FILE=REGISTRY SSS FUL L1
L6              STR

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY -  AVAILABLE VIA OFFLINE PRINT *

Structure attributes must be viewed using STN Express query preparation.
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L14            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  L8 AND BEILSTEIN/LC NOT
                 CAPLUS/LC
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L23           29 SEA FILE=BEILSTEIN ABB=ON  PLU=ON  L22 AND BABSAN/FA
L25            1 SEA FILE=BEILSTEIN ABB=ON  PLU=ON  L14
L26           10 SEA FILE=BEILSTEIN ABB=ON  PLU=ON  L22 NOT L23
L27            8 SEA FILE=BEILSTEIN ABB=ON  PLU=ON  L26 AND RN/FA
L28            2 SEA FILE=BEILSTEIN ABB=ON  PLU=ON  L26 NOT L27
L29            3 SEA FILE=BEILSTEIN ABB=ON  PLU=ON  L25 OR L28


=> file babs
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FILE COVERS 1980 TO DATE.

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                  OR 5924807/BABSAN OR 6073136/BABSAN OR 6308281/BABSAN)


=> dup rem L9 L11 L13 L17 L18 L29 L24
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PROCESSING COMPLETED FOR L9
PROCESSING COMPLETED FOR L11
PROCESSING COMPLETED FOR L13
PROCESSING COMPLETED FOR L17
PROCESSING COMPLETED FOR L18
PROCESSING COMPLETED FOR L29
PROCESSING COMPLETED FOR L24
L80          22 DUP REM L9 L11 L13 L17 L18 L29 L24 (9 DUPLICATES REMOVED)
                ANSWERS '1-15' FROM FILE ZCAPLUS
                ANSWER '16' FROM FILE PROUSDDR
                ANSWER '17' FROM FILE SYNTHLINE
                ANSWERS '18-20' FROM FILE BEILSTEIN
                ANSWERS '21-22' FROM FILE BABS

=> d ibib abs hitstr L80 1-15; d iall L80 16-17; d ide allref L80 18-20; d iall L80
21-22

L80  ANSWER 1 OF 22  ZCAPLUS  COPYRIGHT 2008 ACS on STN DUPLICATE 1
ACCESSION NUMBER:         2006:605352  ZCAPLUS  Full-text
DOCUMENT NUMBER:          145:83371
TITLE:                    Preparation of prodrug constructs of pyrimidinone
                          compounds as calcilytics
INVENTOR(S):              Shcherbakova, Irina; Wermuth, Camille G.; Jeannot,
                          Frederic; Ciapetti, Paola; Roques, Virginie; Jung,
                          Laetitia M.; Balandrin, Manuel F.; Nair, Satheesh, K.;
                          Swierczek, Krzysztof; McCaffrey, Jennifer; Heaton,
                          William L.; Breinholt, Jeff A.; Conklin, Rebecca L.
PATENT ASSIGNEE(S):       NPS Pharmaceuticals, Inc., USA
SOURCE:                   PCT Int. Appl., 53 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.          KIND   DATE        APPLICATION NO.        DATE
     ----------------    ----   --------    --------------------   --------
     WO 2006066070        A2    20060622    WO 2005-US45565        20051216
     WO 2006066070        A3    20060921
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR,
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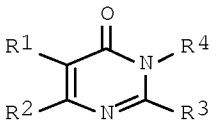
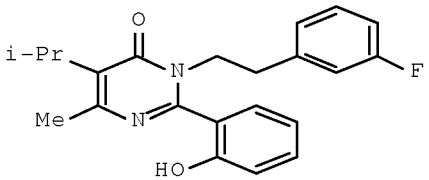
KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX,
MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE,
SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC,
VN, YU, ZA, ZM, ZW
RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
KG, KZ, MD, RU, TJ, TM

PRIORITY APPLN. INFO.: US 2004-637115P P 20041217
OTHER SOURCE(S): MARPAT 145:83371
GI



I

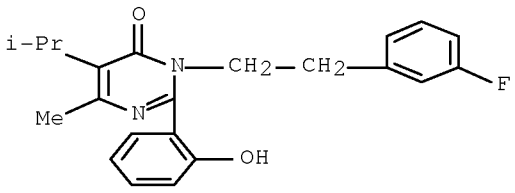


II

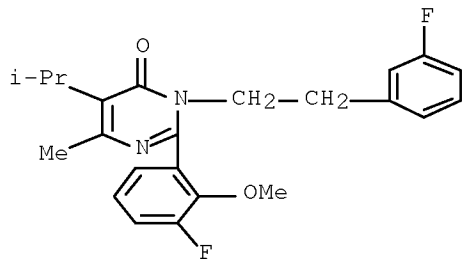
AB Calcilytic pyrimidinones I [R1 and R2 = H, halo, CN, CF3, etc.; R3 = (un)substituted aryl group; R4 = H, alkyl, aryl, etc.], and prodrugs as well as pharmaceutically acceptable salts thereof, are prepared for use in treating disease or disorders characterized by abnormal bone or mineral homeostasis. Thus, e.g., II was prepared by amidation of anisoyl chloride with 2-amino-2-isopropylbut-2-enoic acid Me ester (preparation given) followed by cyclization with 3-fluorphenethyl amine and demethylation. Calcilytic compds. are compds. capable of inhibiting calcium receptor activity. Assays for determining calcium receptor inhibition are described with parameter of desirable IC50 values given. Methods for preparing these compds., oral bioavailability of these compds., pharmaceutical compns. containing these compds. and their use as calcium receptor antagonists are also disclosed.

IT 780771-48-4P 893053-18-4P 893053-34-4P
893054-04-1P 893054-20-1P 893054-36-9P
893054-44-9P 893054-51-8P 893054-67-6P
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of prodrug constructs of pyrimidinone compound as calcilytics)

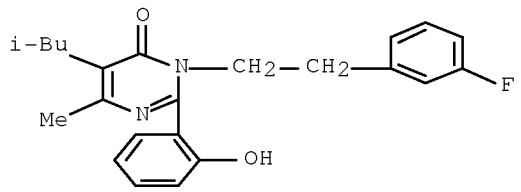
RN 780771-48-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-5-(1-methylethyl)- (CA INDEX NAME)



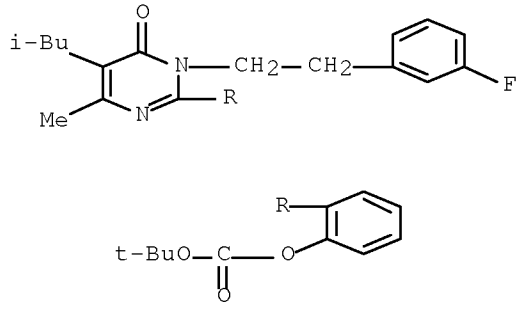
RN 893053-18-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-methoxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl-5-(1-methylethyl)- (CA INDEX NAME)



RN 893053-34-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-5-(2-methylpropyl)- (CA INDEX NAME)

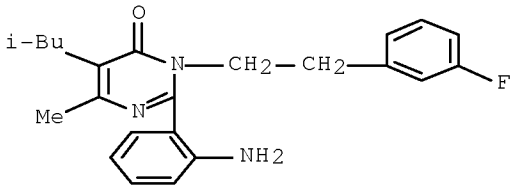


RN 893054-04-1 ZCAPLUS
CN Carbonic acid, 1,1-dimethylethyl 2-[1-[2-(3-fluorophenyl)ethyl]-1,6-dihydro-4-methyl-5-(2-methylpropyl)-6-oxo-2-pyrimidinyl]phenyl ester (9CI) (CA INDEX NAME)

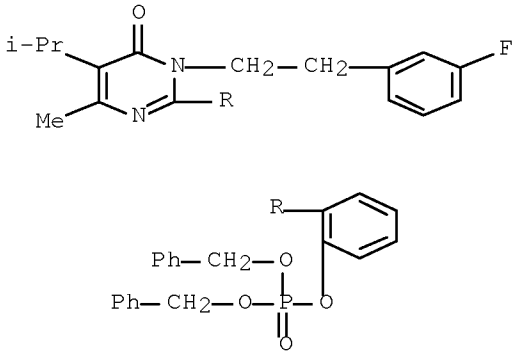


RN 893054-20-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-aminophenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl-

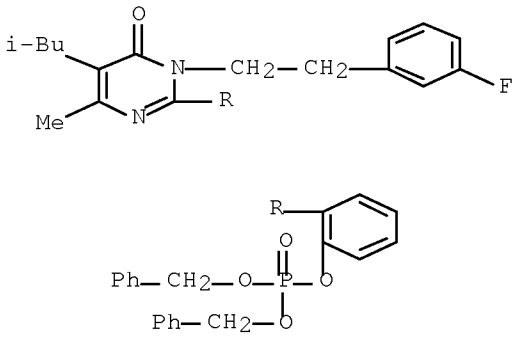
5-(2-methylpropyl)- (CA INDEX NAME)



RN 893054-36-9 ZCAPLUS
CN Phosphoric acid, 2-[1-[2-(3-fluorophenyl)ethyl]-1,6-dihydro-4-methyl-5-(1-methylethyl)-6-oxo-2-pyrimidinyl]phenyl bis(phenylmethyl) ester (CA INDEX NAME)

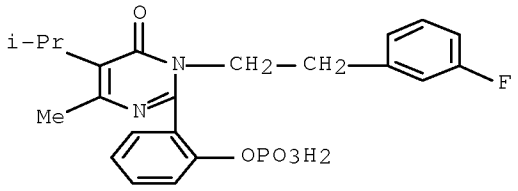


RN 893054-44-9 ZCAPLUS
CN Phosphoric acid, 2-[1-[2-(3-fluorophenyl)ethyl]-1,6-dihydro-4-methyl-5-(2-methylpropyl)-6-oxo-2-pyrimidinyl]phenyl bis(phenylmethyl) ester (CA INDEX NAME)

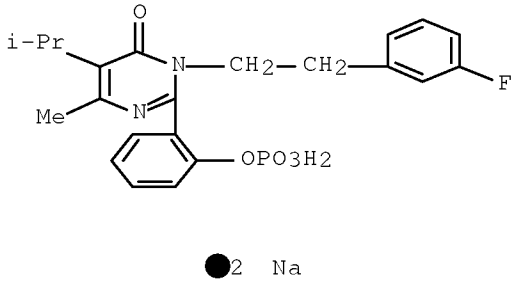


RN 893054-51-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-6-methyl-5-(1-methylethyl)-

2-[2-(phosphonooxy)phenyl]- (9CI) (CA INDEX NAME)



RN 893054-67-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-6-methyl-5-(1-methylethyl)-2-[2-(phosphonooxy)phenyl]-, disodium salt (9CI) (CA INDEX NAME)



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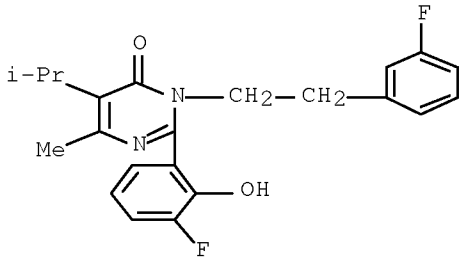
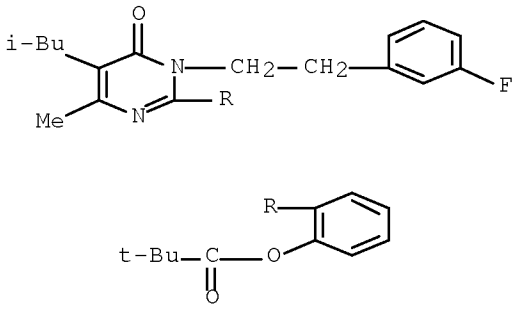
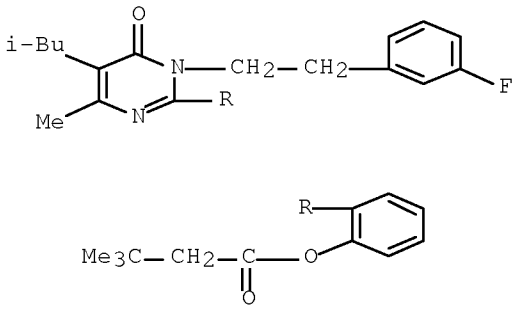
893053-81-1P 893053-88-8P 893053-96-8P
893054-12-1P 893054-28-9P 893054-59-6P
893054-75-6P
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of prodrug constructs of pyrimidinone compound as calcilytics)
RN 893053-26-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl-5-(1-methylethyl)- (CA INDEX NAME)



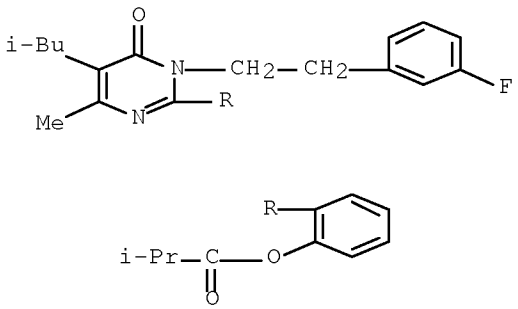
RN 893053-42-4 ZCAPLUS
CN Propanoic acid, 2,2-dimethyl-, 2-[1-[2-(3-fluorophenyl)ethyl]-1,6-dihydro-4-methyl-5-(2-methylpropyl)-6-oxo-2-pyrimidinyl]phenyl ester (CA INDEX NAME)



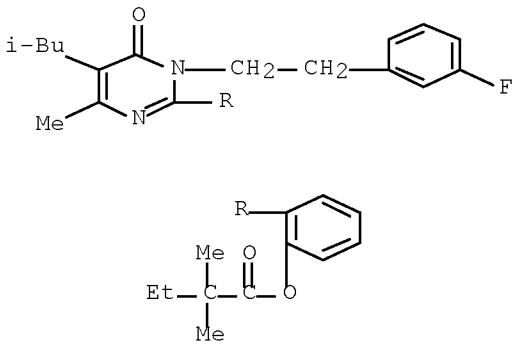
RN 893053-50-4 ZCAPLUS
CN Butanoic acid, 3,3-dimethyl-, 2-[1-[2-(3-fluorophenyl)ethyl]-1,6-dihydro-4-methyl-5-(2-methylpropyl)-6-oxo-2-pyrimidinyl]phenyl ester (CA INDEX NAME)



RN 893053-57-1 ZCAPLUS
CN Propanoic acid, 2-methyl-, 2-[1-[2-(3-fluorophenyl)ethyl]-1,6-dihydro-4-methyl-5-(2-methylpropyl)-6-oxo-2-pyrimidinyl]phenyl ester (CA INDEX NAME)

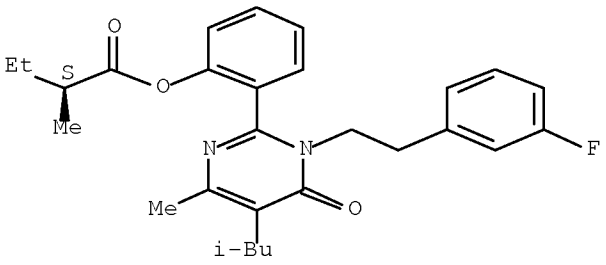


RN 893053-65-1 ZCAPLUS
CN Butanoic acid, 2,2-dimethyl-, 2-[1-[2-(3-fluorophenyl)ethyl]-1,6-dihydro-4-methyl-5-(2-methylpropyl)-6-oxo-2-pyrimidinyl]phenyl ester (CA INDEX NAME)

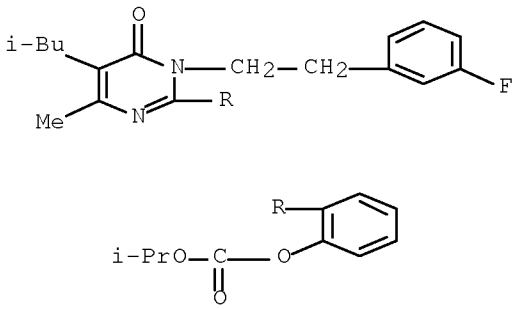


RN 893053-73-1 ZCAPLUS
CN Butanoic acid, 2-methyl-, 2-[1-[2-(3-fluorophenyl)ethyl]-1,6-dihydro-4-methyl-5-(2-methylpropyl)-6-oxo-2-pyrimidinyl]phenyl ester, (2S)- (CA INDEX NAME)

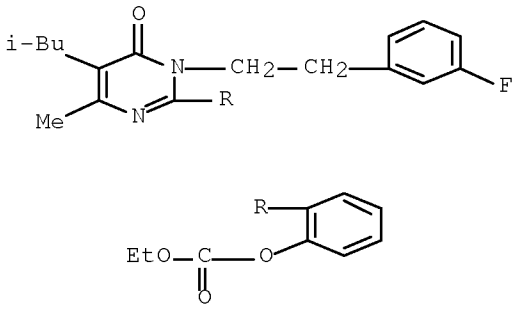
Absolute stereochemistry.



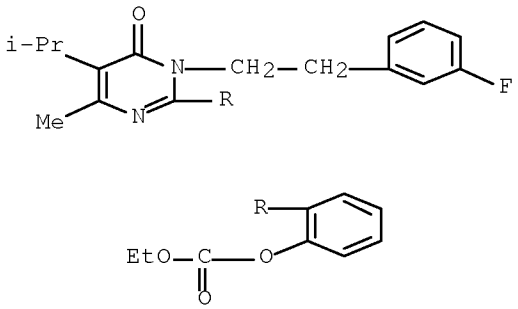
RN 893053-81-1 ZCAPLUS
CN Carbonic acid, 2-[1-[2-(3-fluorophenyl)ethyl]-1,6-dihydro-4-methyl-5-(2-methylpropyl)-6-oxo-2-pyrimidinyl]phenyl 1-methylethyl ester (CA INDEX NAME)



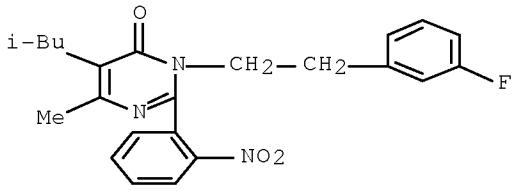
RN 893053-88-8 ZCAPLUS
CN Carbonic acid, ethyl 2-[1-[2-(3-fluorophenyl)ethyl]-1,6-dihydro-4-methyl-5-(2-methylpropyl)-6-oxo-2-pyrimidinyl]phenyl ester (9CI) (CA INDEX NAME)



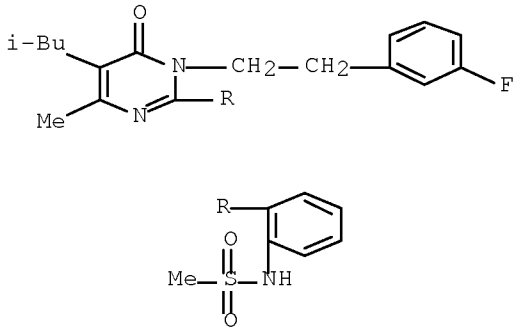
RN 893053-96-8 ZCAPLUS
CN Carbonic acid, ethyl 2-[1-[2-(3-fluorophenyl)ethyl]-1,6-dihydro-4-methyl-5-(1-methylethyl)-6-oxo-2-pyrimidinyl]phenyl ester (9CI) (CA INDEX NAME)



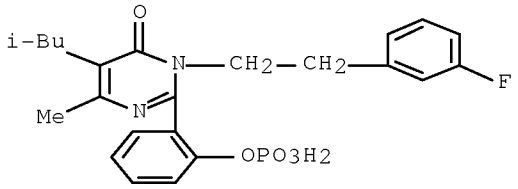
RN 893054-12-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-6-methyl-5-(2-methylpropyl)-2-(2-nitrophenyl)- (CA INDEX NAME)



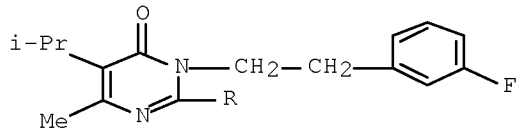
RN 893054-28-9 ZCAPLUS
CN Methanesulfonamide, N-[2-[1-[2-(3-fluorophenyl)ethyl]-1,6-dihydro-4-methyl-5-(2-methylpropyl)-6-oxo-2-pyrimidinyl]phenyl]- (CA INDEX NAME)

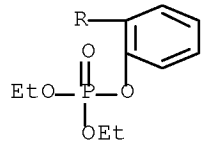


RN 893054-59-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-6-methyl-5-(2-methylpropyl)-2-[2-(phosphonooxy)phenyl]- (9CI) (CA INDEX NAME)

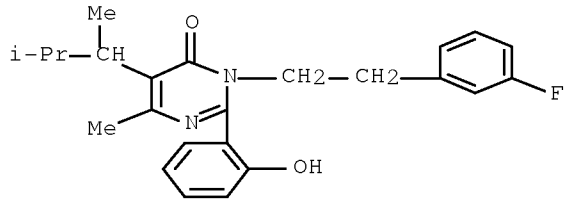


RN 893054-75-6 ZCAPLUS
CN Phosphoric acid, diethyl 2-[1-[2-(3-fluorophenyl)ethyl]-1,6-dihydro-4-methyl-5-(1-methylethyl)-6-oxo-2-pyrimidinyl]phenyl ester (9CI) (CA INDEX NAME)

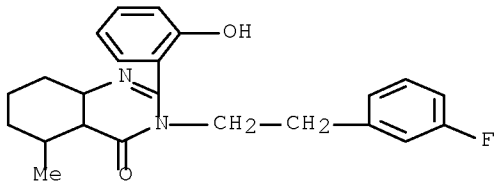




IT 893054-83-6P 893054-91-6P 893054-99-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of prodrug constructs of pyrimidinone compound as calcilytics)
RN 893054-83-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(1,2-dimethylpropyl)-3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl- (CA INDEX NAME)

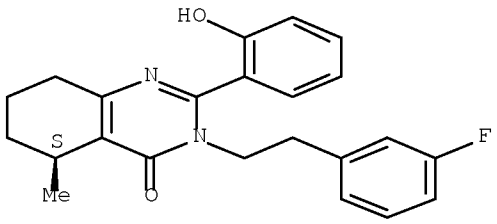


RN 893054-91-6 ZCAPLUS
CN 4(3H)-Quinazolinone, 3-[2-(3-fluorophenyl)ethyl]-4a,5,6,7,8,8a-hexahydro-2-(2-hydroxyphenyl)-5-methyl- (CA INDEX NAME)

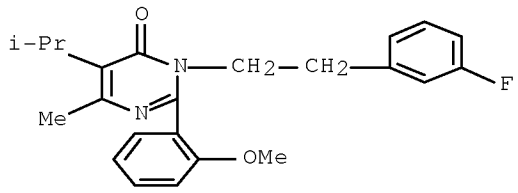


RN 893054-99-4 ZCAPLUS
CN 4(3H)-Quinazolinone, 3-[2-(3-fluorophenyl)ethyl]-5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)-5-methyl-, (5S)- (CA INDEX NAME)

Absolute stereochemistry.



IT 780771-51-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of prodrug constructs of pyrimidinone compound as calcilytics)
RN 780771-51-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-2-(2-methoxyphenyl)-6-methyl-5-(1-methylethyl)- (CA INDEX NAME)



L80 ANSWER 2 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 2
ACCESSION NUMBER: 2005:378882 ZCAPLUS Full-text
DOCUMENT NUMBER: 143:59927
TITLE: Design, new synthesis, and calcilytic activity of substituted 3H-pyrimidin-4-ones
AUTHOR(S): Shcherbakova, Irina; Huang, Guangfei; Geoffroy, Otto J.; Nair, Satheesh K.; Swierczek, Krzysztof; Balandrin, Manuel F.; Fox, John; Heaton, William L.; Conklin, Rebecca L.
CORPORATE SOURCE: Drug Discovery, NPS Pharmaceuticals, Inc., Salt Lake City, UT, 84108, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(10), 2537-2540
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 143:59927
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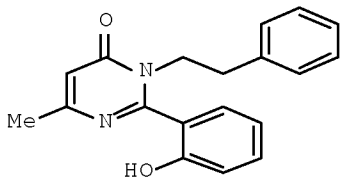
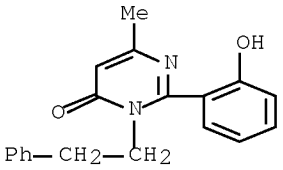


I

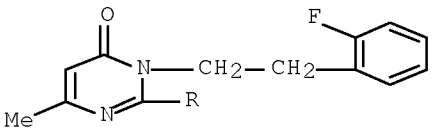
AB Design, synthesis, structure-activity relationship studies and calcium receptor antagonist (calcilytic) properties of 3H-pyrimidin-4-ones, e.g., I, are described. The pyrimidinones were synthesized by multistep procedures.

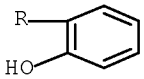
IT 780771-32-6P 780771-33-7P 780771-34-8P
780771-35-9P 780771-41-7P 780771-43-9P
780771-44-0P 780771-47-3P 780771-48-4P
780771-53-1P 780771-54-2P 780771-55-3P
780771-56-4P 780771-57-5P 780771-58-6P
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation, calcilytic activity, and structure-activity relationship of substituted pyrimidinones starting from hydroxybenzonitrile or β-keto esters and phenylethylamines using multistep procedures)

RN 780771-32-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)

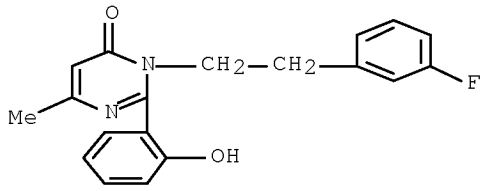


RN 780771-33-7 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(2-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl- (CA INDEX NAME)

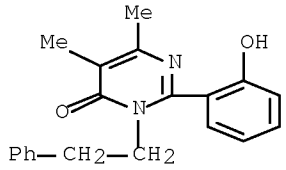




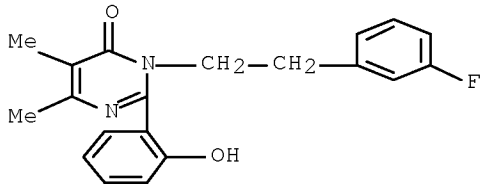
RN 780771-34-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl- (CA INDEX NAME)



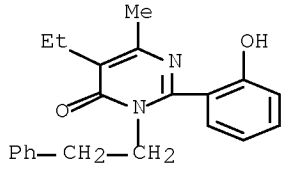
RN 780771-35-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-5,6-dimethyl-3-(2-phenylethyl)-
(CA INDEX NAME)



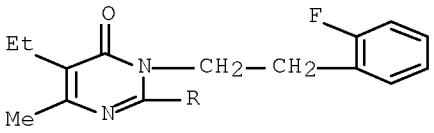
RN 780771-41-7 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5,6-
dimethyl- (CA INDEX NAME)

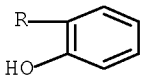


RN 780771-43-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)-
(CA INDEX NAME)

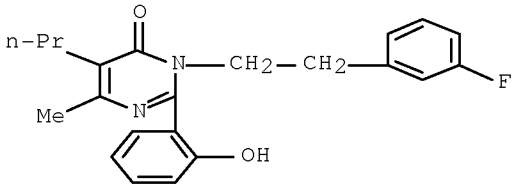


RN 780771-44-0 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-3-[2-(2-fluorophenyl)ethyl]-2-(2-
hydroxyphenyl)-6-methyl- (CA INDEX NAME)

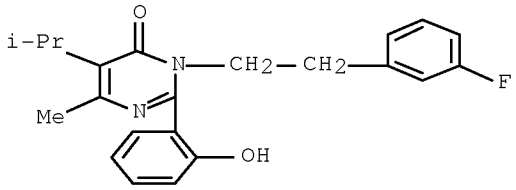




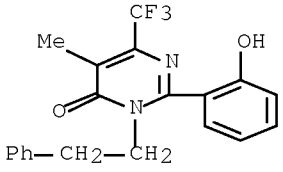
RN 780771-47-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-5-propyl- (CA INDEX NAME)



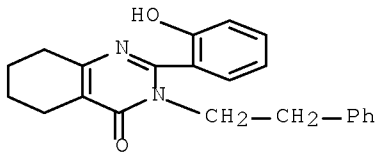
RN 780771-48-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-5-(1-methylethyl)- (CA INDEX NAME)



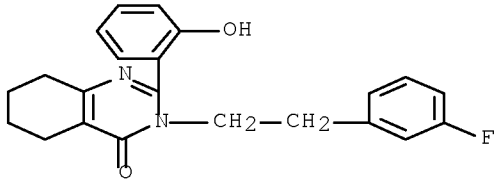
RN 780771-53-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-5-methyl-3-(2-phenylethyl)-6-(trifluoromethyl)- (CA INDEX NAME)



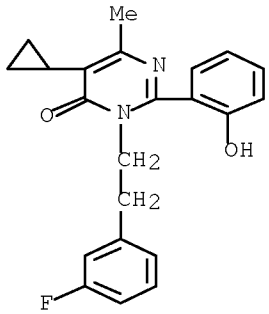
RN 780771-54-2 ZCAPLUS
CN 4(3H)-Quinazolinone, 5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)-3-(2-phenylethyl)- (CA INDEX NAME)



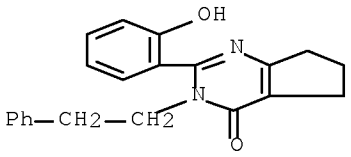
RN 780771-55-3 ZCAPLUS
CN 4(3H)-Quinazolinone, 3-[2-(3-fluorophenyl)ethyl]-5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)- (CA INDEX NAME)



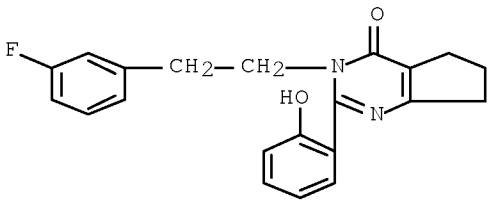
RN 780771-56-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-cyclopropyl-3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl- (CA INDEX NAME)



RN 780771-57-5 ZCAPLUS
CN 4H-Cyclopentapyrimidin-4-one, 3,5,6,7-tetrahydro-2-(2-hydroxyphenyl)-3-(2-phenylethyl)- (9CI) (CA INDEX NAME)



RN 780771-58-6 ZCAPLUS
CN 4H-Cyclopentapyrimidin-4-one, 3-[2-(3-fluorophenyl)ethyl]-3,5,6,7-tetrahydro-2-(2-hydroxyphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L80 ANSWER 3 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 3
ACCESSION NUMBER: 2004:902339 ZCAPLUS Full-text
DOCUMENT NUMBER: 141:379934
TITLE: Preparation of 2,3,5,6-tetrasubstituted 3H-pyrimidin-4-ones via cyclization of carboxamides.
INVENTOR(S): Shcherbakova, Irina; Balandrin, Manuel; Huang, Guangfei; Geoffroy, Otto; Fox, John; Nair, Satheesh K.
PATENT ASSIGNEE(S): NPS Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 33 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004092121	A2	20041028	WO 2004-US10639	20040407
WO 2004092121	A3	20050414		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1613606	A2	20060111	EP 2004-749815	20040407

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR

JP 2006522160	T	20060928	JP 2006-509759		20040407
US 20070161792	A1	20070712	US 2006-551920		20061120
PRIORITY APPLN. INFO.:			US 2003-460859P	P	20030407
			US 2003-479323P	P	20030618
			WO 2004-US10639	W	20040407

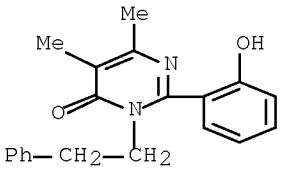
OTHER SOURCE(S): CASREACT 141:379934; MARPAT 141:379934

AB The title process is claimed. Thus, 3-(2-acetoxybenzoylamino)-2-methylbut- 2-enoic acid phenethylamide (preparation given) was refluxed overnight with KOH in EtOH/H2O to give 37% 2-(2-hydroxyphenyl)-5,6-dimethyl-3-phenethyl-3H-pyrimidin-4-one.

IT 780771-35-9P 780771-40-6P 780771-41-7P
780771-42-8P 780771-43-9P 780771-44-0P
780771-45-1P 780771-46-2P 780771-47-3P
780771-48-4P 780771-51-9P 780771-52-0P
780771-54-2P 780771-55-3P 780771-56-4P
780771-57-5P 780771-58-6P 916335-88-1P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(preparation of tetrasubstituted pyrimidinones via cyclization of carboxamides)

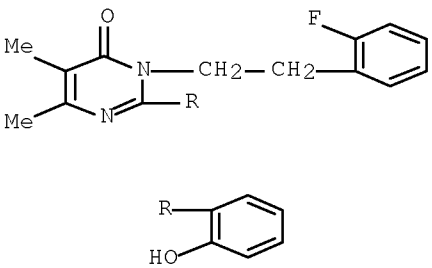
RN 780771-35-9 ZCAPLUS

CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-5,6-dimethyl-3-(2-phenylethyl)- (CA INDEX NAME)



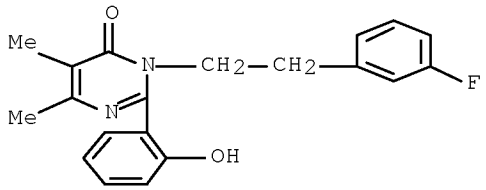
RN 780771-40-6 ZCAPLUS

CN 4(3H)-Pyrimidinone, 3-[2-(2-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5,6-dimethyl- (CA INDEX NAME)

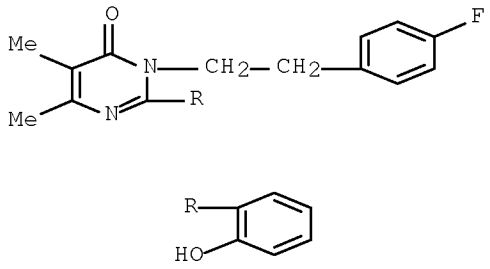


RN 780771-41-7 ZCAPLUS

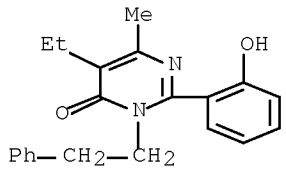
CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5,6-dimethyl- (CA INDEX NAME)



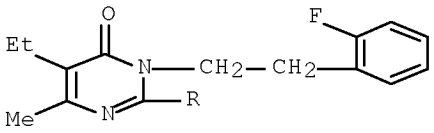
RN 780771-42-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(4-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5,6-dimethyl- (CA INDEX NAME)

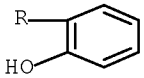


RN 780771-43-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)

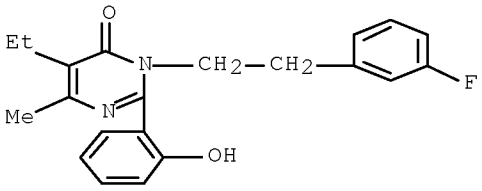


RN 780771-44-0 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-3-[2-(2-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl- (CA INDEX NAME)

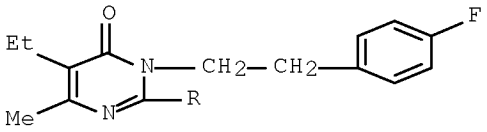


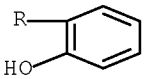


RN 780771-45-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl- (CA INDEX NAME)

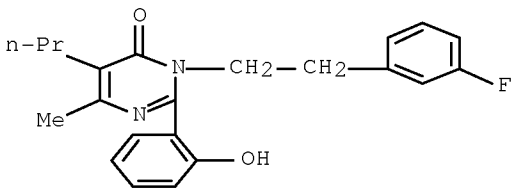


RN 780771-46-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-3-[2-(4-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl- (CA INDEX NAME)

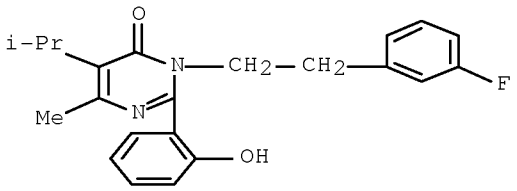




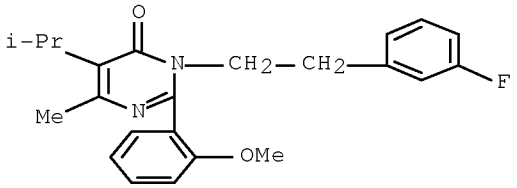
RN 780771-47-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-5-propyl- (CA INDEX NAME)



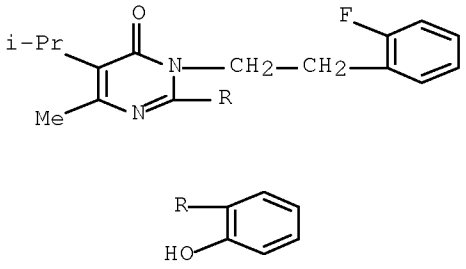
RN 780771-48-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-5-(1-methylethyl)- (CA INDEX NAME)



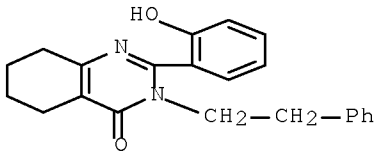
RN 780771-51-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-2-(2-methoxyphenyl)-6-methyl-5-(1-methylethyl)- (CA INDEX NAME)



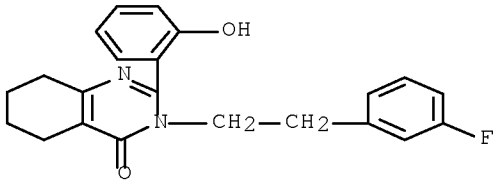
RN 780771-52-0 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(2-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-5-(1-methylethyl)- (CA INDEX NAME)



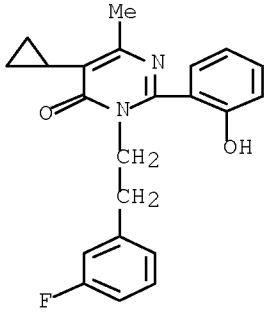
RN 780771-54-2 ZCAPLUS
CN 4(3H)-Quinazolinone, 5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)-3-(2-phenylethyl)- (CA INDEX NAME)



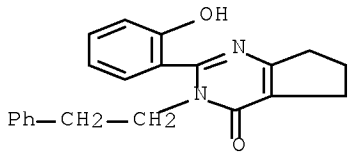
RN 780771-55-3 ZCAPLUS
CN 4(3H)-Quinazolinone, 3-[2-(3-fluorophenyl)ethyl]-5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)- (CA INDEX NAME)



RN 780771-56-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-cyclopropyl-3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl- (CA INDEX NAME)

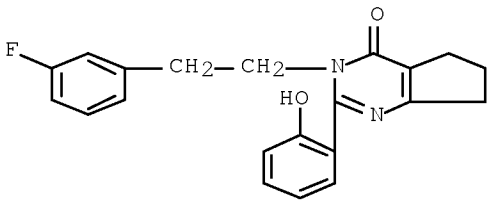


RN 780771-57-5 ZCAPLUS
CN 4H-Cyclopentapyrimidin-4-one, 3,5,6,7-tetrahydro-2-(2-hydroxyphenyl)-3-(2-phenylethyl)- (9CI) (CA INDEX NAME)

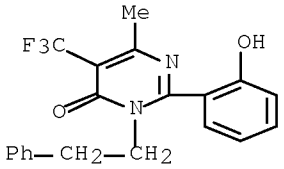


RN 780771-58-6 ZCAPLUS

CN 4H-Cyclopentapyrimidin-4-one, 3-[2-(3-fluorophenyl)ethyl]-3,5,6,7-tetrahydro-2-(2-hydroxyphenyl)- (9CI) (CA INDEX NAME)



RN 916335-88-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)-5-(trifluoromethyl)- (CA INDEX NAME)



L80 ANSWER 4 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 4
ACCESSION NUMBER: 2004:902338 ZCAPLUS Full-text
DOCUMENT NUMBER: 141:366249
TITLE: Preparation of pyrimidinone compounds as calcilytics
INVENTOR(S): Shcherbakova, Irina V.; Balandrin, Manuel F.; Huang, Guangfei; Geoffroy, Otto; Fox, John; Marquis, Robert; Yamashita, Dennis Shinji; Luengo, Juan; Wang, Wenyong
PATENT ASSIGNEE(S): NPS Pharmaceuticals, Inc., USA; Glaxosmithkline
SOURCE: PCT Int. Appl., 57 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004092120	A2	20041028	WO 2004-US10638	20040407
WO 2004092120	A3	20050414		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,

SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2004230903	A1	20041028	AU 2004-230903		20040407
CA 2521129	A1	20041028	CA 2004-2521129		20040407
EP 1615897	A2	20060118	EP 2004-749814		20040407
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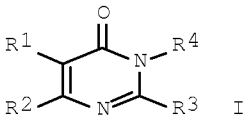
CN 1835928	A	20060920	CN 2004-80009255		20040407
JP 2006522159	T	20060928	JP 2006-509758		20040407
MX 2005PA10683	A	20060801	MX 2005-PA10683		20051004
US 20070197555	A1	20070823	US 2006-552363		20061120
PRIORITY APPLN. INFO.:			US 2003-460859P	P	20030407
			US 2003-479323P	P	20030618
			WO 2004-US10638	W	20040407

OTHER SOURCE(S): CASREACT 141:366249; MARPAT 141:366249

GI



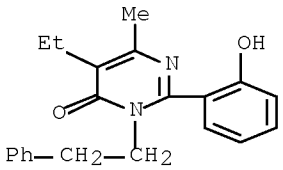
I

AB Title compds. I [R1-2 = H, halo, CN, CF3, etc.; R3 = aryl; R4 = H, alkyl, etc.] are prepared For instance, 2-(2-Hydroxyphenyl)-6-methyl-3-phenethyl-3H-pyrimidin-4-one is prepared from o-hydroxybenzonitrile, acetyl chloride and Me acetoacetate. Compds. of the invention have IC50 values < 30 μM in a calcium receptor inhibition assay. I are useful for the treatment of abnormal bone or mineral homeostasis.

IT 780771-43-9P, 5-Ethyl-2-(2-hydroxyphenyl)-6-methyl-3-phenethyl-3H-pyrimidin-4-one 780771-51-9P, 3-[2-(3-Fluorophenyl)ethyl]-5-isopropyl-2-(2-methoxyphenyl)-6-methyl-3H-pyrimidin-4-one
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of pyrimidinone compds. as calcilytics)

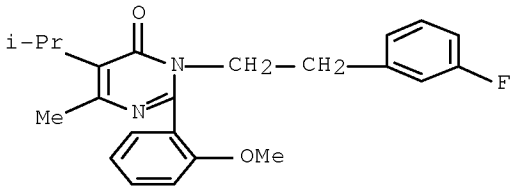
RN 780771-43-9 ZCAPLUS

CN 4(3H)-Pyrimidinone, 5-ethyl-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



RN 780771-51-9 ZCAPLUS

CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-2-(2-methoxyphenyl)-6-methyl-5-(1-methylethyl)- (CA INDEX NAME)



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fluorophenyl)ethyl]-2-(2-hydroxy-4-methoxyphenyl)-6-methyl-3H-pyrimidin-4-one
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of pyrimidinone compds. as calcilytics)

RN 780771-32-6 ZCAPLUS
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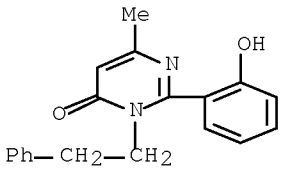
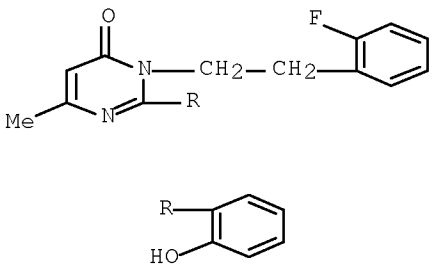
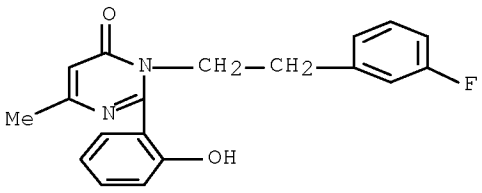


RN 780771-33-7 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(2-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl- (CA INDEX NAME)



RN 780771-34-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl- (CA INDEX NAME)



RN 780771-35-9 ZCAPLUS
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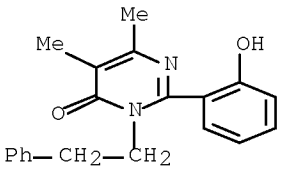
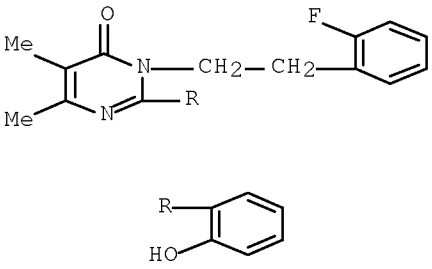
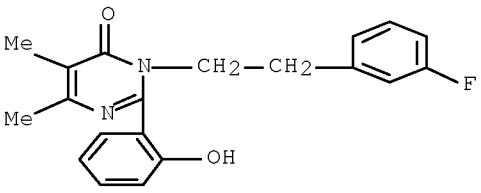


RN 780771-40-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(2-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5,6-dimethyl- (CA INDEX NAME)



RN 780771-41-7 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-5,6-dimethyl- (CA INDEX NAME)



RN 780771-42-8 ZCAPLUS
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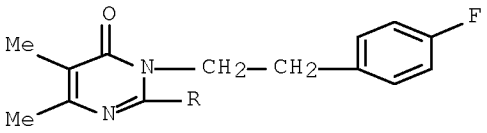

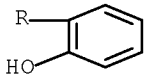

RN 780771-44-0 ZCAPLUS
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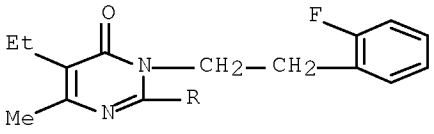

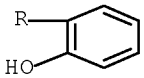

RN 780771-45-1 ZCAPLUS
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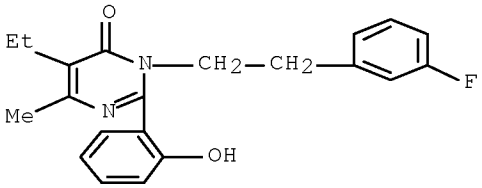

RN 780771-46-2 ZCAPLUS
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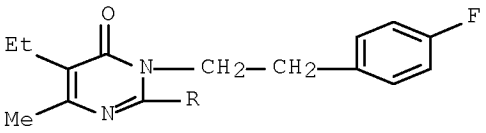

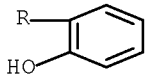

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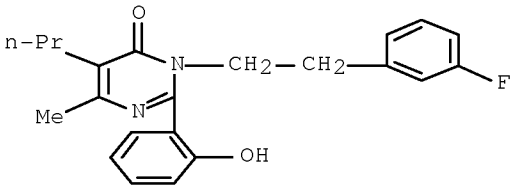

RN 780771-48-4 ZCAPLUS
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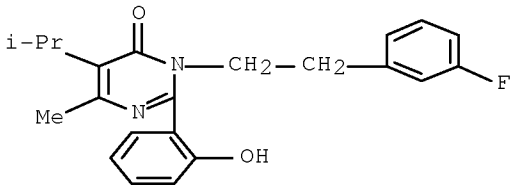

RN 780771-52-0 ZCAPLUS
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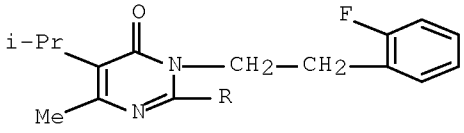
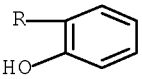
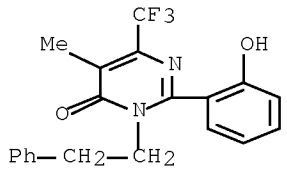




RN 780771-53-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-5-methyl-3-(2-phenylethyl)-6-(trifluoromethyl)- (CA INDEX NAME)



RN 780771-54-2 ZCAPLUS
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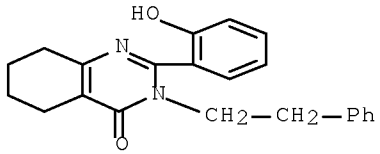

RN 780771-55-3 ZCAPLUS
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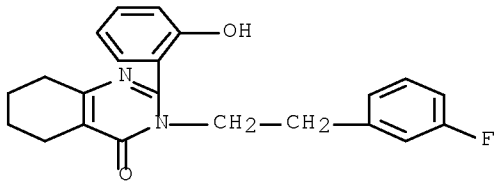

RN 780771-56-4 ZCAPLUS
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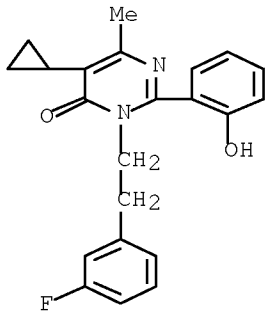

RN 780771-57-5 ZCAPLUS
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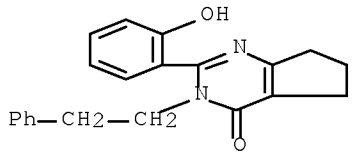

RN 780771-58-6 ZCAPLUS
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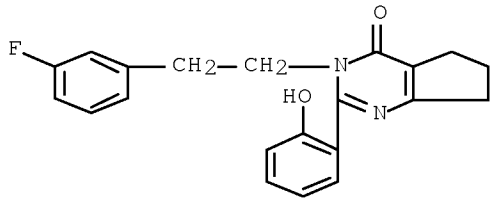

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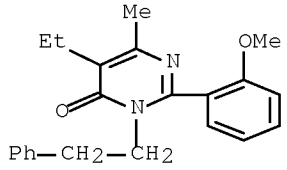
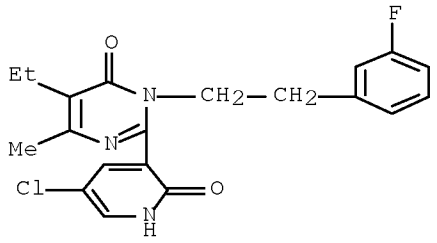
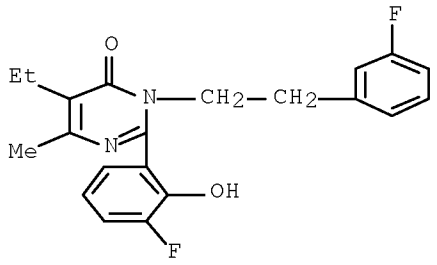


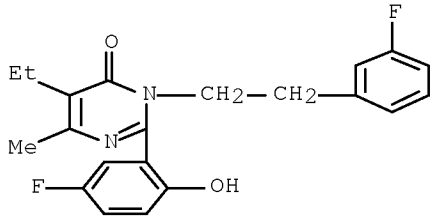
RN 780771-60-0 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(5-chloro-1,2-dihydro-2-oxo-3-pyridinyl)-5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl- (CA INDEX NAME)



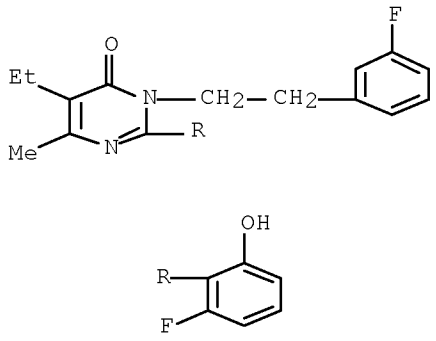
RN 780771-62-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-2-(3-fluoro-2-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl- (CA INDEX NAME)



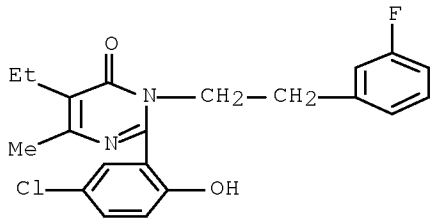
RN 780771-64-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-2-(5-fluoro-2-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl- (CA INDEX NAME)



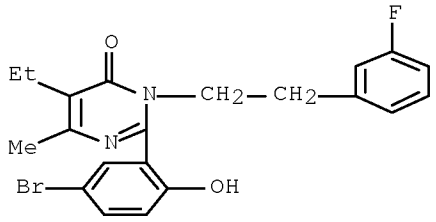
RN 780771-65-5 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-2-(2-fluoro-6-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl- (CA INDEX NAME)



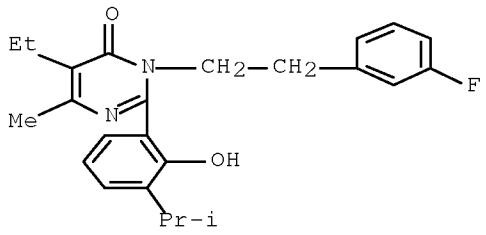
RN 780771-67-7 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(5-chloro-2-hydroxyphenyl)-5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl- (CA INDEX NAME)



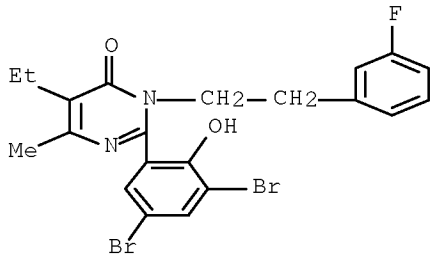
RN 780771-68-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(5-bromo-2-hydroxyphenyl)-5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl- (CA INDEX NAME)



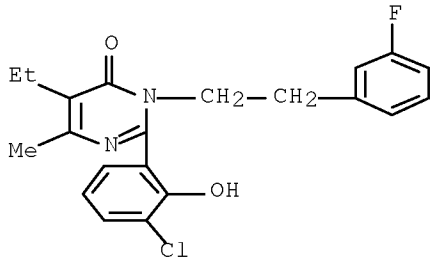
RN 780771-69-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-3-[2-(3-fluorophenyl)ethyl]-2-[2-hydroxy-3-(1-methylethyl)phenyl]-6-methyl- (CA INDEX NAME)



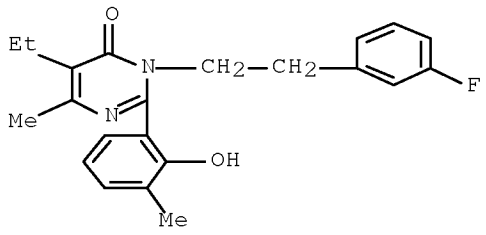
RN 780771-71-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3,5-dibromo-2-hydroxyphenyl)-5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl- (CA INDEX NAME)



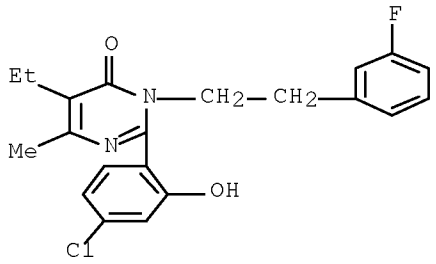
RN 780771-72-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-chloro-2-hydroxyphenyl)-5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl- (CA INDEX NAME)



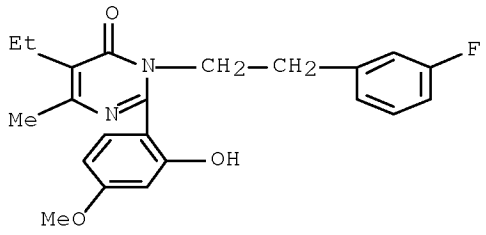
RN 780771-74-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxy-3-methylphenyl)-6-methyl- (CA INDEX NAME)



RN 780771-75-7 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(4-chloro-2-hydroxyphenyl)-5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl- (CA INDEX NAME)



RN 780771-76-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxy-4-methoxyphenyl)-6-methyl- (CA INDEX NAME)



L80 ANSWER 5 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 5
ACCESSION NUMBER: 2001:574517 ZCAPLUS Full-text
DOCUMENT NUMBER: 135:344327
TITLE: [2+2] Cycloaddition reactions of 1-benzyl-2,4-diphenyl-1,3-diazabuta-1,3-diene with chiral ketenes
AUTHOR(S): Abbiati, G.; Rossi, E.
CORPORATE SOURCE: Istituto di Chimica Organica della Facolta di Farmacia, Universita di Milano, Milan, I-20133, Italy
SOURCE: Tetrahedron (2001), 57(33), 7205-7212
CODEN: TETRAB; ISSN: 0040-4020

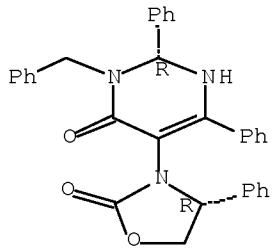
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:344327

AB The [2+2] cycloaddn. reactions of 1-benzyl-2,4-diphenyl-1,3-diaza-1,3-butadiene [i.e., N'-(phenylmethyl)-N-(phenylmethylene)benzenecarboximidami de] with β-(dimethylphenylsilyl)ketene, β-menthoxyketene and Evans-Sjogren ketene were investigated. The results and some chemical transformations of the obtained cycloadducts are reported.

IT 371961-79-4P 371961-81-8P 371961-82-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

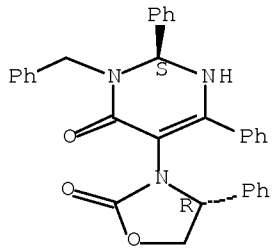
RN 371961-79-4 ZCAPLUS
CN 4(1H)-Pyrimidinone, 2,3-dihydro-5-[(4R)-2-oxo-4-phenyl-3-oxazolidinyl]-2,6-diphenyl-3-(phenylmethyl)-, (2R)- (CA INDEX NAME)

Absolute stereochemistry.



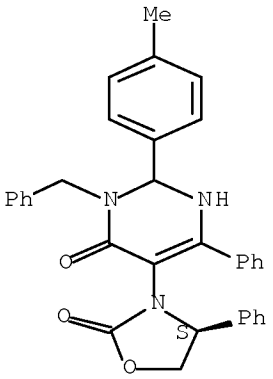
RN 371961-81-8 ZCAPLUS
CN 4(1H)-Pyrimidinone, 2,3-dihydro-5-[(4R)-2-oxo-4-phenyl-3-oxazolidinyl]-2,6-diphenyl-3-(phenylmethyl)-, (2S)- (CA INDEX NAME)

Absolute stereochemistry.



RN 371961-82-9 ZCAPLUS
CN 4(1H)-Pyrimidinone, 2,3-dihydro-2-(4-methylphenyl)-5-[(4S)-2-oxo-4-phenyl-3-oxazolidinyl]-6-phenyl-3-(phenylmethyl)- (CA INDEX NAME)

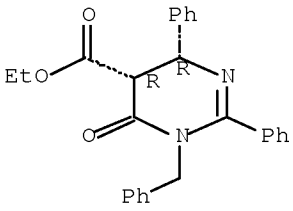
Absolute stereochemistry.



REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

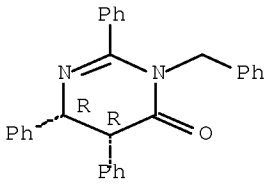
L80 ANSWER 6 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 6
ACCESSION NUMBER: 1997:681277 ZCAPLUS Full-text
DOCUMENT NUMBER: 127:358828
ORIGINAL REFERENCE NO.: 127:70247a,70250a
TITLE: [4+2] and [2+2] Cycloaddition reactions of 1-(4-methylphenyl) and 1-benzyl-1,3-diaza-1,3-butadienes with ketenes
AUTHOR(S): Rossi, Elisabetta; Abbiati, Giorgio; Pini, Elena
CORPORATE SOURCE: Istituto di Chimica Organica, Facolta di Farmacia, Universita degli Studi di Milano, Milan, I-20133, Italy
SOURCE: Tetrahedron (1997), 53(41), 14107-14114
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB [4+2] And [2+2] Cycloaddn. reactions of 1-(4-methylphenyl) and 1-benzyl-1,3-diaza-1,3-butadienes with monophenyl, di-Ph, monochloro and ethoxycarbonylketenes are described. The mechanism of these reactions is also discussed.
IT 198630-83-0P 198630-84-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(cycloaddn. of (methylphenyl) and benzyl-diazabutadienes with ketenes)
RN 198630-83-0 ZCAPLUS
CN 5-Pyrimidinecarboxylic acid, 1,4,5,6-tetrahydro-6-oxo-2,4-diphenyl-1-(phenylmethyl)-, ethyl ester, (4R,5R)-rel- (CA INDEX NAME)

Relative stereochemistry.



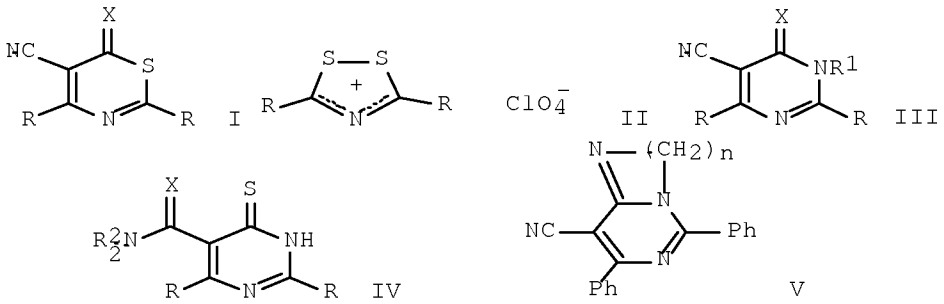
RN 198630-84-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5,6-dihydro-2,5,6-triphenyl-3-(phenylmethyl)-, (5R,6R)-rel- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L80 ANSWER 7 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN DUPLICATE 7
ACCESSION NUMBER: 1995:92361 ZCAPLUS Full-text
DOCUMENT NUMBER: 122:55981
ORIGINAL REFERENCE NO.: 122:10847a,10850a
TITLE: Synthesis of N-substituted oxo- and thioxopyrimidines from 1,2,4-dithiazolium salts
AUTHOR(S): Holzer, Max; Dobner, Bodo; Briel, Detlef
CORPORATE SOURCE: Fakultoet Biowissenschaften, Pharmazie Psychologie, Universitaet Leipzig, Leipzig, D-04103, Germany
SOURCE: Liebigs Annalen der Chemie (1994), (9), 901-9
CODEN: LACHDL; ISSN: 0170-2041
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 122:55981
GI

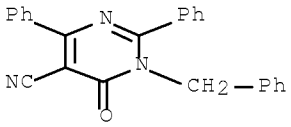


AB 2,4-Diaryl-substituted 1,3-thiazine-5-carbonitriles I (X = O, S, R = aryl), obtained by reaction of 1,2,4-dithiazolium salts II with activated cyanoacetates, undergo ring transformations in the presence of primary and secondary amines. Thus, I react with primary amines, R1NH2, under mild conditions to give hardly accessible N-3-substituted oxopyrimidine- or thioxopyrimidine-5-carbonitriles III and with secondary amines, R22NH, to give N-3-unsubstituted pyrimidine derivs. IV and with diamines to give imidazo[1,2-

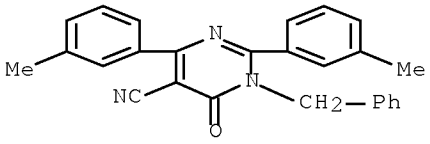
c]pyrimidines or pyrimido[1,2-c]pyrimidines V (n = 2,3). After alkylation of 1,3-thiazines I, highly reactive 1,3-thiazinium salts 8 can be isolated.

IT 159851-80-6P 159851-86-2P 159851-87-3P
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(Synthesis of N-substituted oxo- and thioxopyrimidines from 1,2,4-dithiazolium salts)

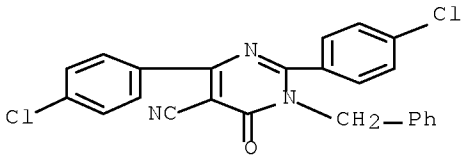
RN 159851-80-6 ZCAPLUS
CN 5-Pyrimidinecarbonitrile, 1,6-dihydro-6-oxo-2,4-diphenyl-1-(phenylmethyl)- (CA INDEX NAME)



RN 159851-86-2 ZCAPLUS
CN 5-Pyrimidinecarbonitrile, 1,6-dihydro-2,4-bis(3-methylphenyl)-6-oxo-1-(phenylmethyl)- (CA INDEX NAME)



RN 159851-87-3 ZCAPLUS
CN 5-Pyrimidinecarbonitrile, 2,4-bis(4-chlorophenyl)-1,6-dihydro-6-oxo-1-(phenylmethyl)- (CA INDEX NAME)



L80 ANSWER 8 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2007:591360 ZCAPLUS Full-text
DOCUMENT NUMBER: 147:31135
TITLE: Pyrimidinone derivatives as calcilytic compounds and their preparation, pharmaceutical compositions and use as calcium receptor inhibitors for treatment of bone and mineral diseases
INVENTOR(S): Ku, Thomas Wen Fu; Lin, Hong; Luengo, Juan I.; Marquis, Robert W., Jr.; Ramanjulu, Joshi M.; Trout, Robert; Yamashita, Dennis S.
PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA

SOURCE: PCT Int. Appl., 251pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

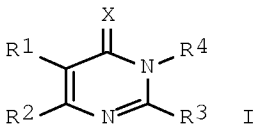
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007062370	A2	20070531	WO 2006-US61150	20061121
WO 2007062370	A3	20071122		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

AU 2006318275	A1	20070531	AU 2006-318275	20061121
PRIORITY APPLN. INFO.:			US 2005-738731P	P 20051122
			US 2005-739067P	P 20051122
			WO 2006-US61150	W 20061121

OTHER SOURCE(S): MARPAT 147:31135
GI



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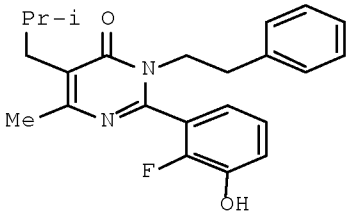


II

AB Novel calcilytic compds. of formula I, pharmaceutical compns., methods of synthesis and methods of using them are provided. Compds. of formula I wherein C is O and S; R1 and R2 are independently H, halo, CN, C1-10 alkyl, C2-6 alkenyl, cycloalkyl, (hetero)aryl, etc.; R3 is (un)substituted (hetero)aryl; R4 is (un)substituted (hetero)aryl, (un)substituted heterocyclyl, (un)substituted cycloalkyl-C1-4 alkyl, etc.; and their pharmaceutically acceptable salts thereof, are claimed. Example compound II was prepared by alkylation of Et 3-oxobutanoate with 3-bromo-2-methyl-1-propene; the resulting Et 2-acetyl-4-methyl-4-pentenoate underwent amidation with phenethylamine to give 2-acetyl-4-methyl-N-(phenethyl)-4- pentenamide, which underwent hydrogenation to give 2-acetyl-4-methyl-N- (phenethyl)-4-pentanamide, which underwent cyclization with 2-fluoro-3-methoxybenzamide to give 2-[2-fluoro-3-methoxyphenyl]-6-methoxy- 5-(2-methylpropyl)-3-(2-phenylethyl)-4(3H)-pyrimidinone, which underwent demethylation to give

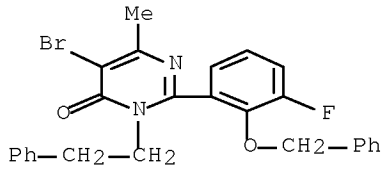
compound II. All the invention compds. were evaluated for their calcium receptor inhibitory activity.

IT 938177-13-0P 938177-15-2P 938177-17-4P
938177-24-3P 938177-37-8P 938177-39-0P
938178-22-4P 938178-61-1P 938179-64-7P
938179-78-3P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate and intermediate; preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)

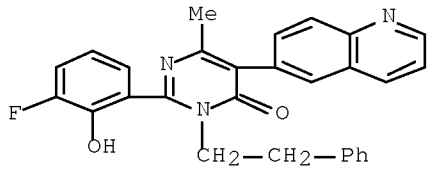
RN 938177-13-0 ZCAPLUS

CN 4(3H)-Pyrimidinone, 5-bromo-2-[3-fluoro-2-(phenylmethoxy)phenyl]-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



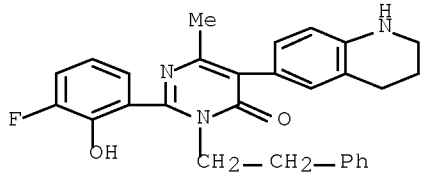
RN 938177-15-2 ZCAPLUS

CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)-5-(6-quinolinyl)- (CA INDEX NAME)



RN 938177-17-4 ZCAPLUS

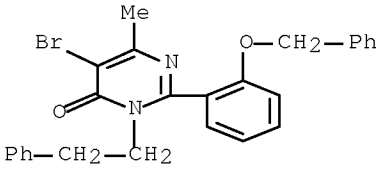
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)-5-(1,2,3,4-tetrahydro-6-quinolinyl)- (CA INDEX NAME)



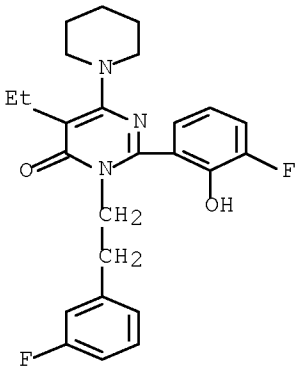
RN 938177-24-3 ZCAPLUS

CN 4(3H)-Pyrimidinone, 5-bromo-6-methyl-3-(2-phenylethyl)-2-[2-

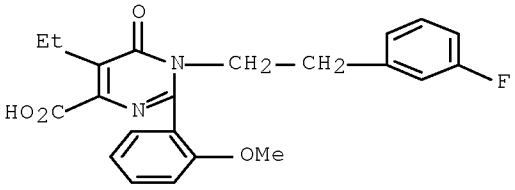
(phenylmethoxy)phenyl]- (CA INDEX NAME)



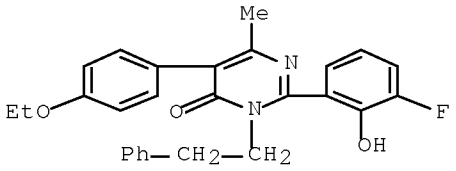
RN 938177-37-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-2-(3-fluoro-2-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-(1-piperidinyl)- (CA INDEX NAME)



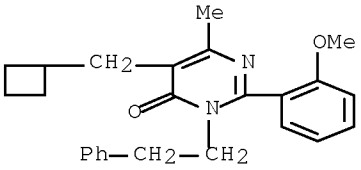
RN 938177-39-0 ZCAPLUS
CN 4-Pyrimidinecarboxylic acid, 5-ethyl-1-[2-(3-fluorophenyl)ethyl]-1,6-dihydro-2-(2-methoxyphenyl)-6-oxo- (CA INDEX NAME)



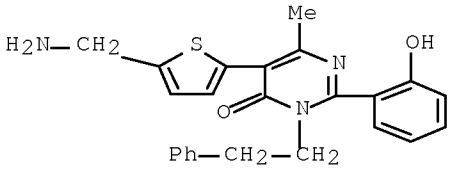
RN 938178-22-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(4-ethoxyphenyl)-2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



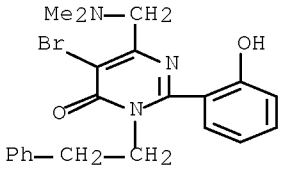
RN 938178-61-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(cyclobutylmethyl)-2-(2-methoxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



RN 938179-64-7 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-[5-(aminomethyl)-2-thienyl]-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



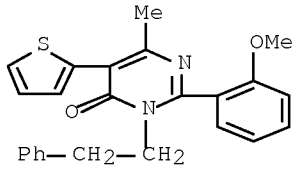
RN 938179-78-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-bromo-6-[(dimethylamino)methyl]-2-(2-hydroxyphenyl)-3-(2-phenylethyl)- (CA INDEX NAME)



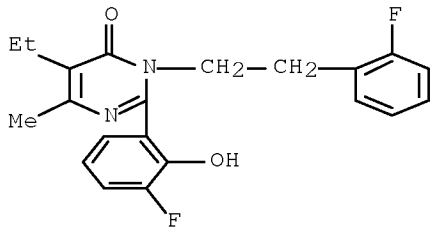
IT 938178-47-3P 938179-15-8P 938179-98-7P
938180-00-8P 938180-13-3P 938180-14-4P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic

preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(drug candidate; preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)

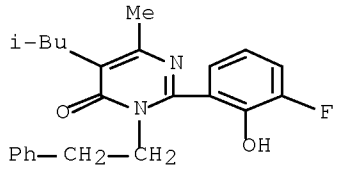
RN 938178-47-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-methoxyphenyl)-6-methyl-3-(2-phenylethyl)-5-(2-thienyl)- (CA INDEX NAME)



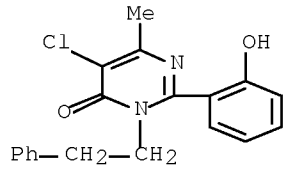
RN 938179-15-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-2-(3-fluoro-2-hydroxyphenyl)-3-[2-(2-fluorophenyl)ethyl]-6-methyl- (CA INDEX NAME)



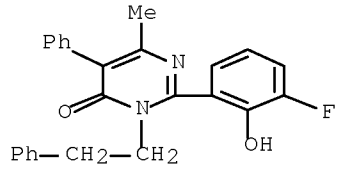
RN 938179-98-7 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-5-(2-methylpropyl)-3-(2-phenylethyl)- (CA INDEX NAME)



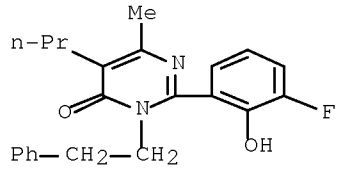
RN 938180-00-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-chloro-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



RN 938180-13-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-5-phenyl-3-(2-phenylethyl)- (CA INDEX NAME)



RN 938180-14-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)-5-propyl- (CA INDEX NAME)



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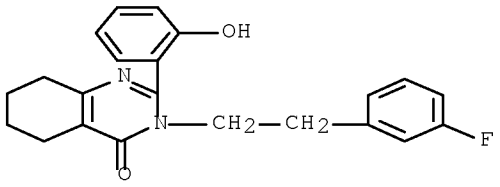
938180-12-2P 938180-15-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

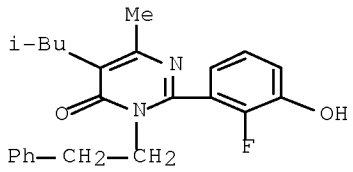
(drug candidate; preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)

RN 780771-55-3 ZCAPLUS

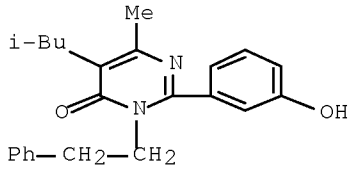
CN 4(3H)-Quinazolinone, 3-[2-(3-fluorophenyl)ethyl]-5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)- (CA INDEX NAME)



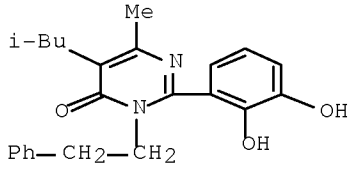
RN 938177-01-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-fluoro-3-hydroxyphenyl)-6-methyl-5-(2-methylpropyl)-3-(2-phenylethyl)- (CA INDEX NAME)



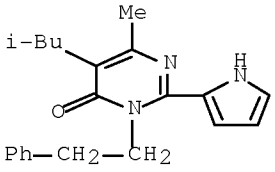
RN 938177-02-7 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-hydroxyphenyl)-6-methyl-5-(2-methylpropyl)-3-(2-phenylethyl)- (CA INDEX NAME)



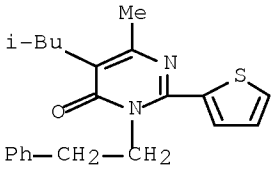
RN 938177-03-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2,3-dihydroxyphenyl)-6-methyl-5-(2-methylpropyl)-3-(2-phenylethyl)- (CA INDEX NAME)



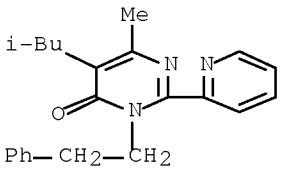
RN 938177-04-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 6-methyl-5-(2-methylpropyl)-3-(2-phenylethyl)-2-(1H-pyrrol-2-yl)- (CA INDEX NAME)



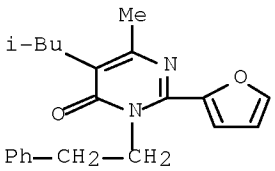
RN 938177-05-0 ZCAPLUS
CN 4(3H)-Pyrimidinone, 6-methyl-5-(2-methylpropyl)-3-(2-phenylethyl)-2-(2-thienyl)- (CA INDEX NAME)



RN 938177-06-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 6-methyl-5-(2-methylpropyl)-3-(2-phenylethyl)-2-(2-pyridinyl)- (CA INDEX NAME)

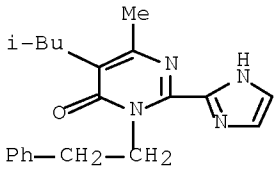


RN 938177-07-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-furanyl)-6-methyl-5-(2-methylpropyl)-3-(2-phenylethyl)- (CA INDEX NAME)



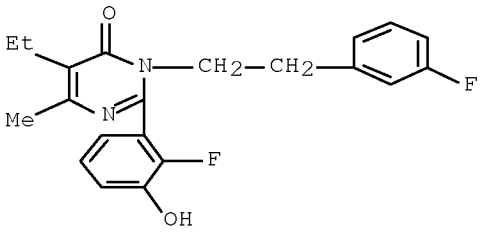
RN 938177-09-4 ZCAPLUS

CN 4(3H)-Pyrimidinone, 2-(1H-imidazol-2-yl)-6-methyl-5-(2-methylpropyl)-3-(2-phenylethyl)- (CA INDEX NAME)



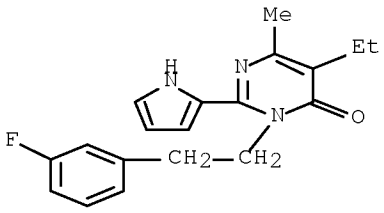
RN 938177-11-8 ZCAPLUS

CN 4(3H)-Pyrimidinone, 5-ethyl-2-(2-fluoro-3-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl- (CA INDEX NAME)



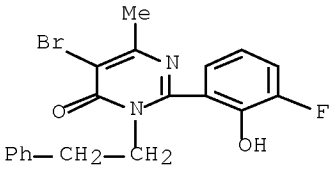
RN 938177-12-9 ZCAPLUS

CN 4(3H)-Pyrimidinone, 5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl-2-(1H-pyrrol-2-yl)- (CA INDEX NAME)

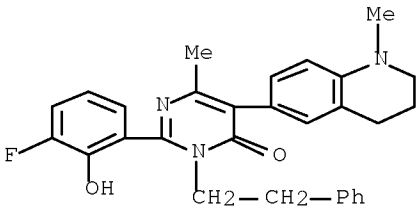


RN 938177-14-1 ZCAPLUS

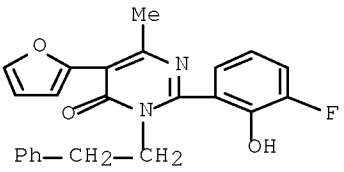
CN 4(3H)-Pyrimidinone, 5-bromo-2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



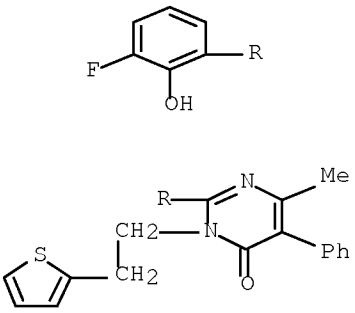
RN 938177-18-5 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)-5-(1,2,3,4-tetrahydro-1-methyl-6-quinolinyl)- (CA INDEX NAME)



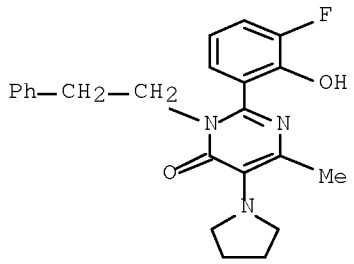
RN 938177-19-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-5-(2-furanyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



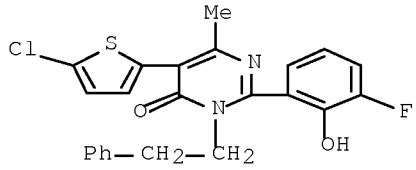
RN 938177-20-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-5-phenyl-3-[2-(2-thienyl)ethyl]- (CA INDEX NAME)



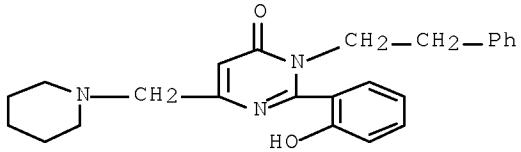
RN 938177-21-0 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)-5-(1-pyrrolidinyl)- (CA INDEX NAME)



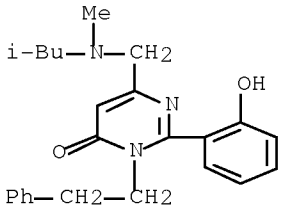
RN 938177-22-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(5-chloro-2-thienyl)-2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



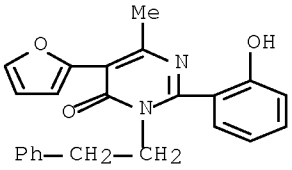
RN 938177-25-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-3-(2-phenylethyl)-6-(1-piperidinylmethyl)- (CA INDEX NAME)



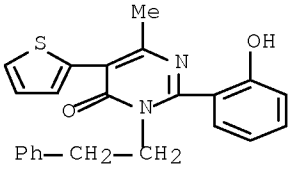
RN 938177-27-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-[[methyl(2-methylpropyl)amino]methyl]-3-(2-phenylethyl)- (CA INDEX NAME)



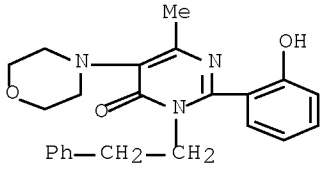
RN 938177-31-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(2-furanyl)-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



RN 938177-33-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)-5-(2-thienyl)- (CA INDEX NAME)



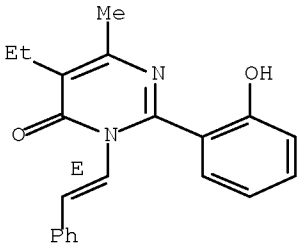
RN 938177-35-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-5-(4-morpholinyl)-3-(2-phenylethyl)- (CA INDEX NAME)



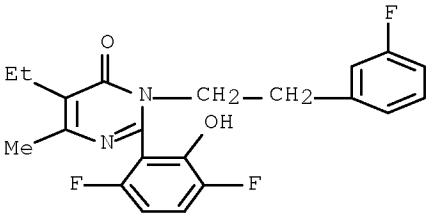
RN 938177-41-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-2-(2-hydroxyphenyl)-6-methyl-3-[(1E)-2-

phenylethenyl]- (CA INDEX NAME)

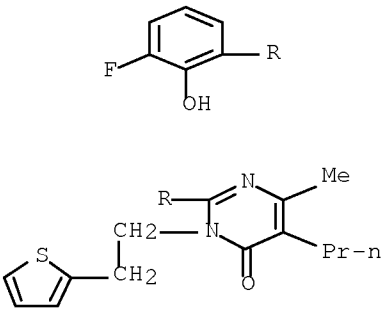
Double bond geometry as shown.



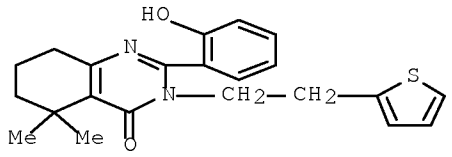
RN 938177-43-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3,6-difluoro-2-hydroxyphenyl)-5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl- (CA INDEX NAME)



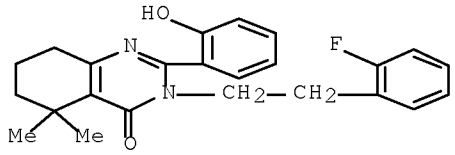
RN 938177-45-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-5-propyl-3-[2-(2-thienyl)ethyl]- (CA INDEX NAME)



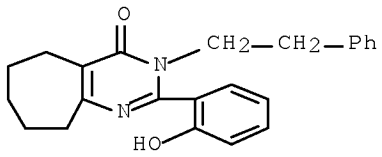
RN 938177-47-0 ZCAPLUS
CN 4(3H)-Quinazolinone, 5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)-5,5-dimethyl-3-[2-(2-thienyl)ethyl]- (CA INDEX NAME)



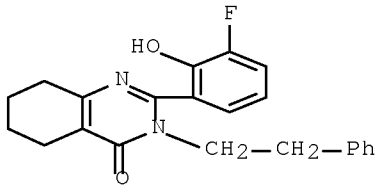
RN 938177-48-1 ZCAPLUS
CN 4(3H)-Quinazolinone, 3-[2-(2-fluorophenyl)ethyl]-5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)-5,5-dimethyl- (CA INDEX NAME)



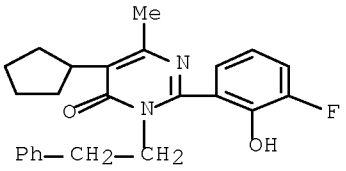
RN 938177-50-5 ZCAPLUS
CN 4H-Cycloheptapyrimidin-4-one, 3,5,6,7,8,9-hexahydro-2-(2-hydroxyphenyl)-3-(2-phenylethyl)- (CA INDEX NAME)



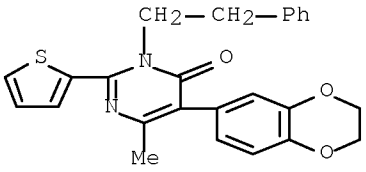
RN 938177-52-7 ZCAPLUS
CN 4(3H)-Quinazolinone, 2-(3-fluoro-2-hydroxyphenyl)-5,6,7,8-tetrahydro-3-(2-phenylethyl)- (CA INDEX NAME)



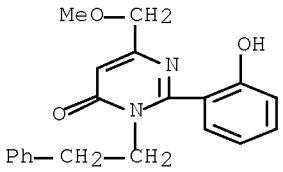
RN 938177-54-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-cyclopentyl-2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



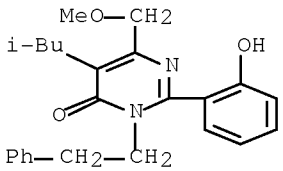
RN 938177-56-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(2,3-dihydro-1,4-benzodioxin-6-yl)-6-methyl-3-(2-phenylethyl)-2-(2-thienyl)- (CA INDEX NAME)



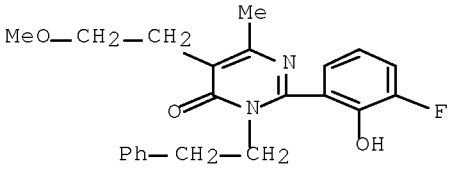
RN 938177-57-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-(methoxymethyl)-3-(2-phenylethyl)- (CA INDEX NAME)



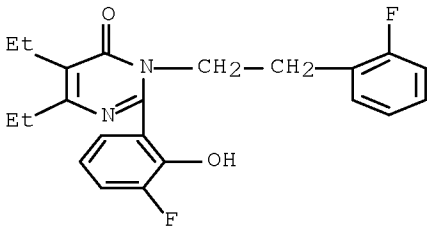
RN 938177-58-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-(methoxymethyl)-5-(2-methylpropyl)-3-(2-phenylethyl)- (CA INDEX NAME)



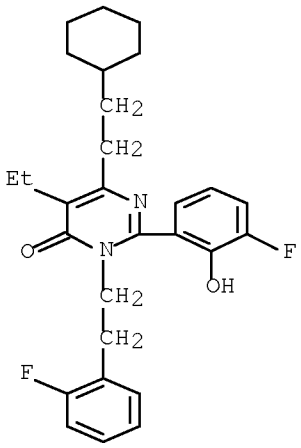
RN 938177-61-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-5-(2-methoxyethyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



RN 938177-71-0 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5,6-diethyl-2-(3-fluoro-2-hydroxyphenyl)-3-[2-(2-fluorophenyl)ethyl]- (CA INDEX NAME)

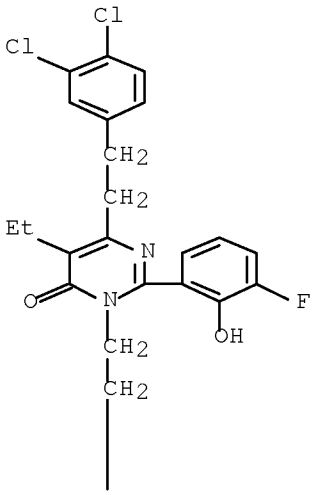


RN 938177-73-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 6-(2-cyclohexylethyl)-5-ethyl-2-(3-fluoro-2-hydroxyphenyl)-3-[2-(2-fluorophenyl)ethyl]- (CA INDEX NAME)

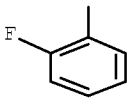


RN 938177-75-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 6-[2-(3,4-dichlorophenyl)ethyl]-5-ethyl-2-(3-fluoro-2-hydroxyphenyl)-3-[2-(2-fluorophenyl)ethyl]- (CA INDEX NAME)

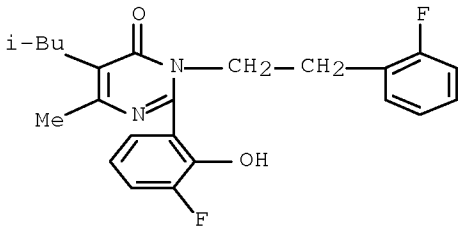
PAGE 1-A



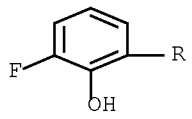
PAGE 2-A

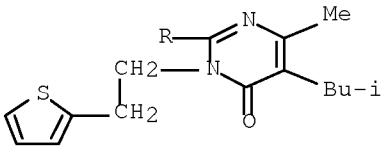


RN 938177-76-5 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-3-[2-(2-fluorophenyl)ethyl]-6-methyl-5-(2-methylpropyl)- (CA INDEX NAME)

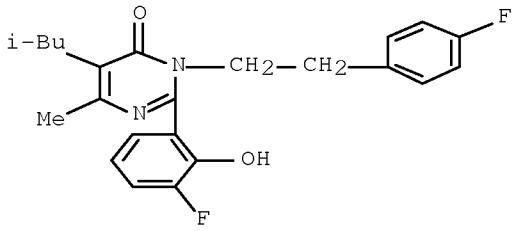


RN 938177-78-7 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-5-(2-methylpropyl)-3-[2-(2-thienyl)ethyl]- (CA INDEX NAME)

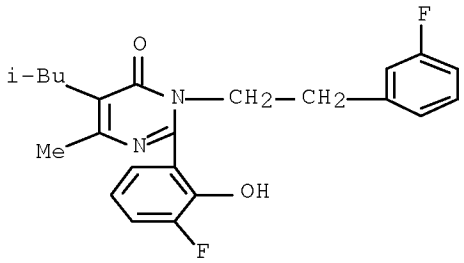




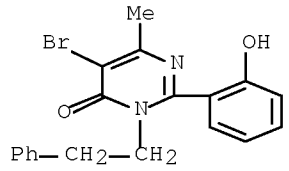
RN 938177-80-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-3-[2-(4-fluorophenyl)ethyl]-6-methyl-5-(2-methylpropyl)- (CA INDEX NAME)



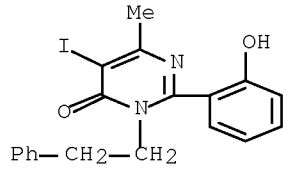
RN 938177-82-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl-5-(2-methylpropyl)- (CA INDEX NAME)



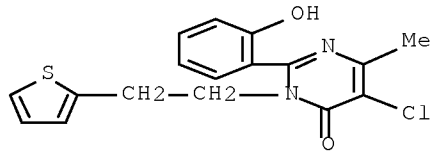
RN 938177-88-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-bromo-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



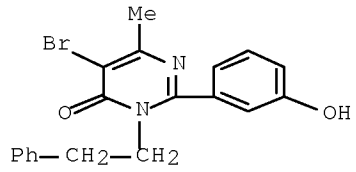
RN 938177-90-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-5-iodo-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



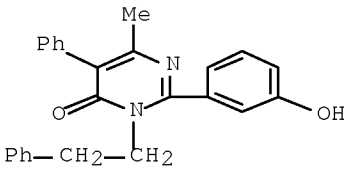
RN 938177-92-5 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-chloro-2-(2-hydroxyphenyl)-6-methyl-3-[2-(2-thienyl)ethyl]- (CA INDEX NAME)



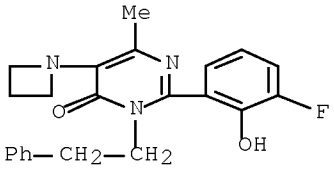
RN 938177-95-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-bromo-2-(3-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



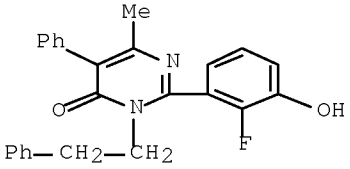
RN 938177-97-0 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-hydroxyphenyl)-6-methyl-5-phenyl-3-(2-phenylethyl)- (CA INDEX NAME)



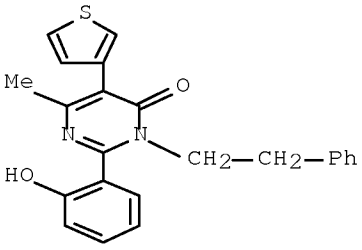
RN 938178-00-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(1-azetidinyl)-2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



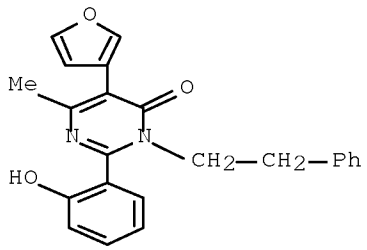
RN 938178-05-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-fluoro-3-hydroxyphenyl)-6-methyl-5-phenyl-3-(2-phenylethyl)- (CA INDEX NAME)



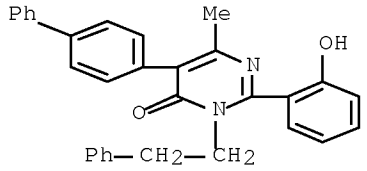
RN 938178-07-5 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)-5-(3-thienyl)- (CA INDEX NAME)



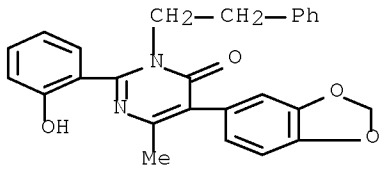
RN 938178-09-7 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(3-furanyl)-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



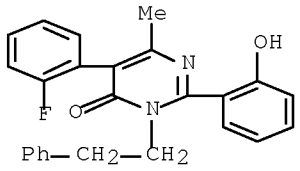
RN 938178-11-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-[1,1'-biphenyl]-4-yl-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



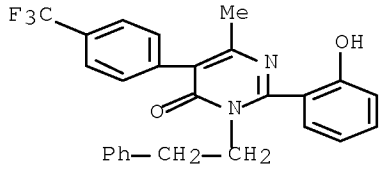
RN 938178-13-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(1,3-benzodioxol-5-yl)-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



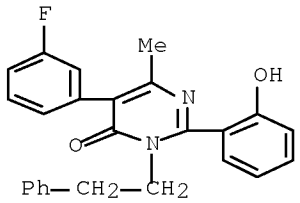
RN 938178-14-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(2-fluorophenyl)-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



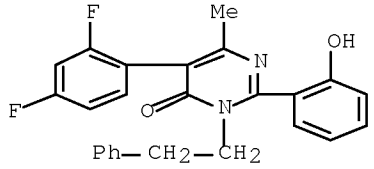
RN 938178-15-5 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)-5-[4-(trifluoromethyl)phenyl]- (CA INDEX NAME)



RN 938178-17-7 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(3-fluorophenyl)-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)

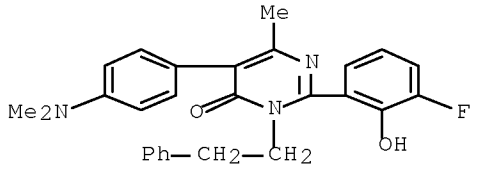


RN 938178-19-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(2,4-difluorophenyl)-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)

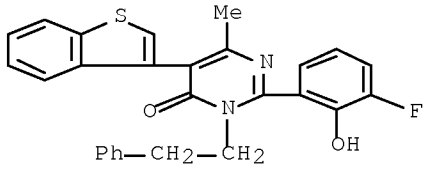


RN 938178-20-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-[4-(dimethylamino)phenyl]-2-(3-fluoro-2-

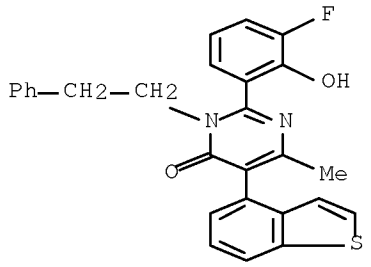
hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



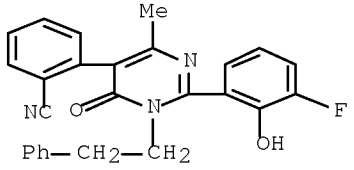
RN 938178-23-5 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-benzo[b]thien-3-yl-2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



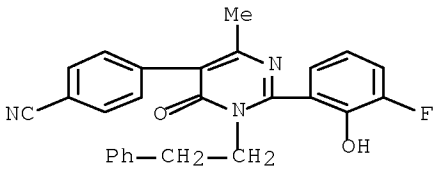
RN 938178-24-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-benzo[b]thien-4-yl-2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



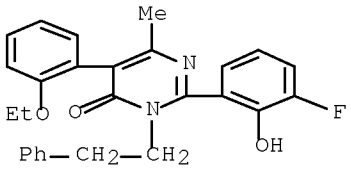
RN 938178-25-7 ZCAPLUS
CN Benzonitrile, 2-[2-(3-fluoro-2-hydroxyphenyl)-1,6-dihydro-4-methyl-6-oxo-1-(2-phenylethyl)-5-pyrimidinyl]- (CA INDEX NAME)



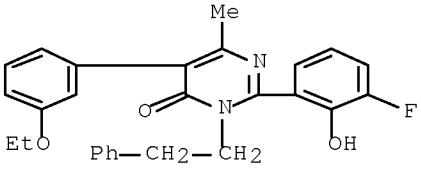
RN 938178-26-8 ZCAPLUS
CN Benzonitrile, 4-[2-(3-fluoro-2-hydroxyphenyl)-1,6-dihydro-4-methyl-6-oxo-1-(2-phenylethyl)-5-pyrimidinyl]- (CA INDEX NAME)



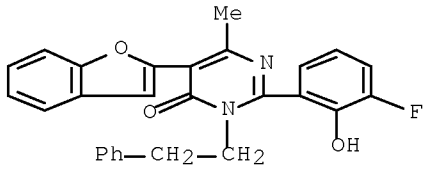
RN 938178-27-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(2-ethoxyphenyl)-2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



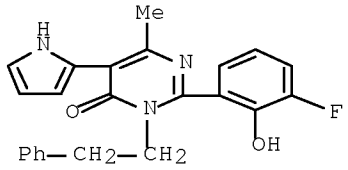
RN 938178-28-0 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(3-ethoxyphenyl)-2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



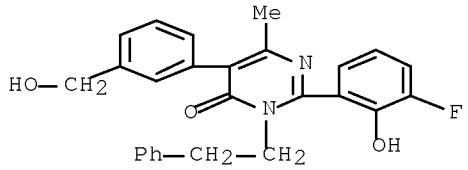
RN 938178-29-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(2-benzofuranyl)-2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



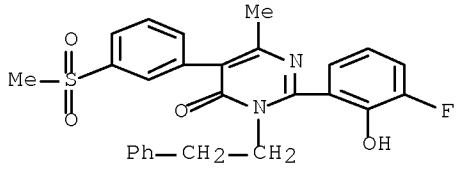
RN 938178-30-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)-5-(1H-pyrrol-2-yl)- (CA INDEX NAME)



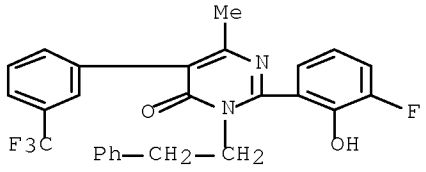
RN 938178-31-5 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-5-[3-(hydroxymethyl)phenyl]-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



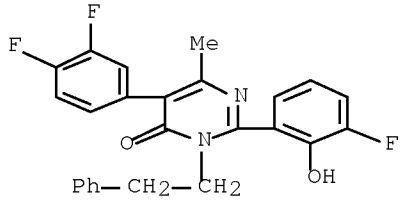
RN 938178-32-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-5-[3-(methylsulfonyl)phenyl]-3-(2-phenylethyl)- (CA INDEX NAME)



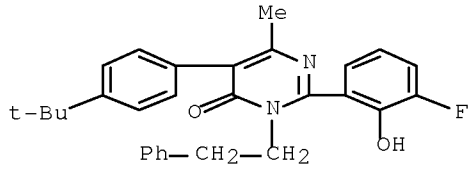
RN 938178-33-7 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)-5-[3-(trifluoromethyl)phenyl]- (CA INDEX NAME)



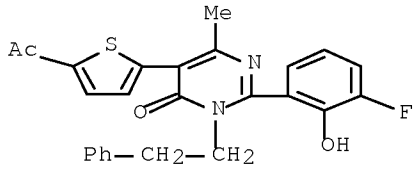
RN 938178-34-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(3,4-difluorophenyl)-2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



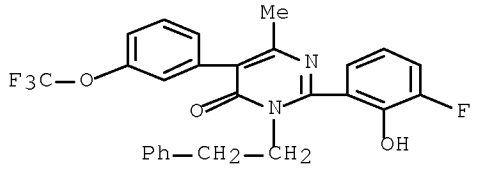
RN 938178-35-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-[4-(1,1-dimethylethyl)phenyl]-2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



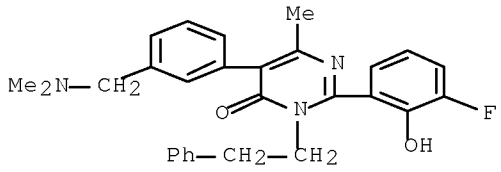
RN 938178-36-0 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(5-acetyl-2-thienyl)-2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



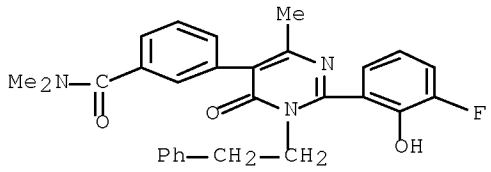
RN 938178-37-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)-5-[3-(trifluoromethoxy)phenyl]- (CA INDEX NAME)



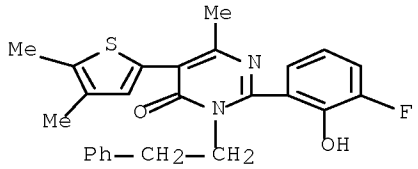
RN 938178-38-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-[3-[(dimethylamino)methyl]phenyl]-2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



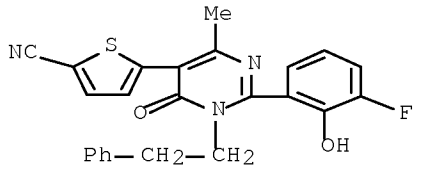
RN 938178-39-3 ZCAPLUS
CN Benzamide, 3-[2-(3-fluoro-2-hydroxyphenyl)-1,6-dihydro-4-methyl-6-oxo-1-(2-phenylethyl)-5-pyrimidinyl]-N,N-dimethyl- (CA INDEX NAME)



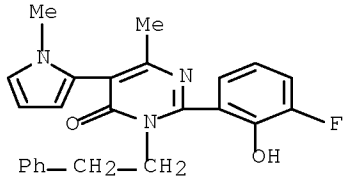
RN 938178-40-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(4,5-dimethyl-2-thienyl)-2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



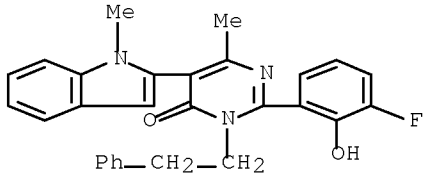
RN 938178-41-7 ZCAPLUS
CN 2-Thiophenecarbonitrile, 5-[2-(3-fluoro-2-hydroxyphenyl)-1,6-dihydro-4-methyl-6-oxo-1-(2-phenylethyl)-5-pyrimidinyl]- (CA INDEX NAME)



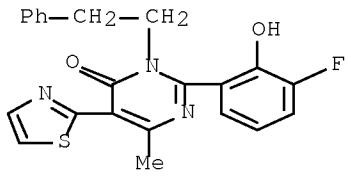
RN 938178-42-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-5-(1-methyl-1H-pyrrol-2-yl)-3-(2-phenylethyl)- (CA INDEX NAME)



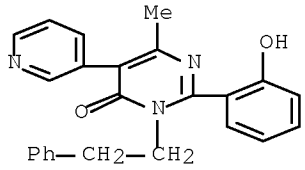
RN 938178-43-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-5-(1-methyl-1H-indol-2-yl)-3-(2-phenylethyl)- (CA INDEX NAME)



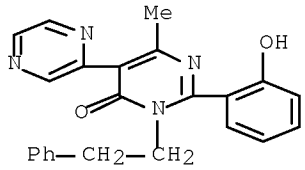
RN 938178-44-0 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)-5-(2-thiazolyl)- (CA INDEX NAME)



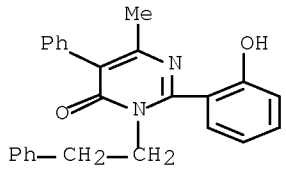
RN 938178-45-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)-5-(3-pyridinyl)- (CA INDEX NAME)



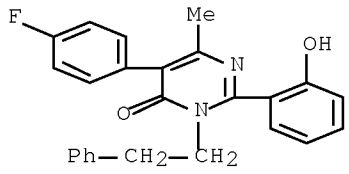
RN 938178-46-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)-5-(2-pyrazinyl)- (CA INDEX NAME)



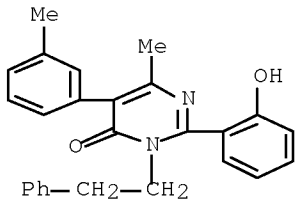
RN 938178-48-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-5-phenyl-3-(2-phenylethyl)- (CA INDEX NAME)



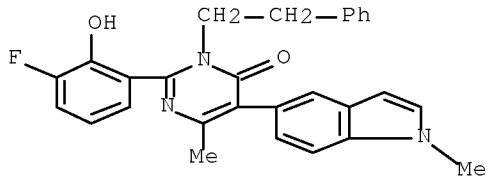
RN 938178-49-5 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(4-fluorophenyl)-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



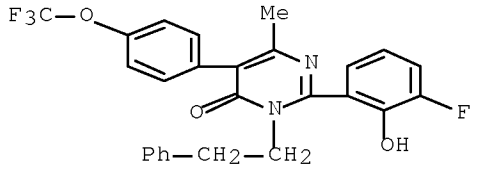
RN 938178-50-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-5-(3-methylphenyl)-3-(2-phenylethyl)- (CA INDEX NAME)



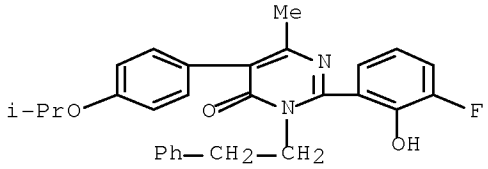
RN 938178-51-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-5-(1-methyl-1H-indol-5-yl)-3-(2-phenylethyl)- (CA INDEX NAME)



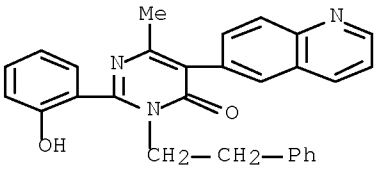
RN 938178-52-0 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)-5-[4-(trifluoromethoxy)phenyl]- (CA INDEX NAME)



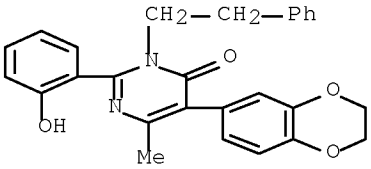
RN 938178-53-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-5-[4-(1-methylethoxy)phenyl]-3-(2-phenylethyl)- (CA INDEX NAME)



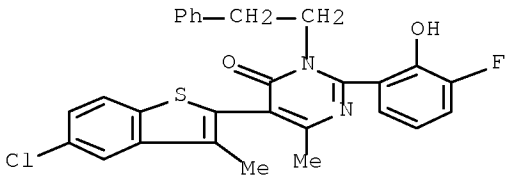
RN 938178-54-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)-5-(6-quinolinyl)- (CA INDEX NAME)



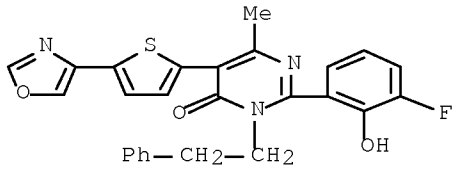
RN 938178-55-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



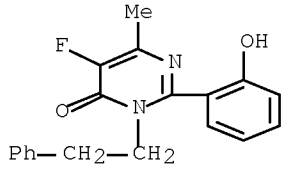
RN 938178-56-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(5-chloro-3-methylbenzo[b]thien-2-yl)-2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



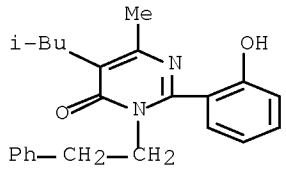
RN 938178-57-5 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-5-[5-(4-oxazolyl)-2-thienyl]-3-(2-phenylethyl)- (CA INDEX NAME)



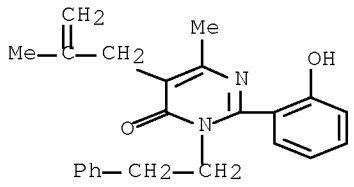
RN 938178-58-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-fluoro-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



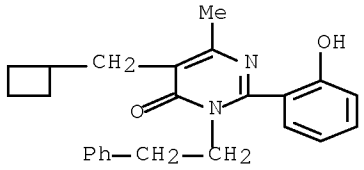
RN 938178-59-7 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-5-(2-methylpropyl)-3-(2-phenylethyl)- (CA INDEX NAME)



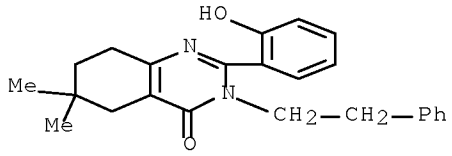
RN 938178-60-0 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-5-(2-methyl-2-propen-1-yl)-3-(2-phenylethyl)- (CA INDEX NAME)



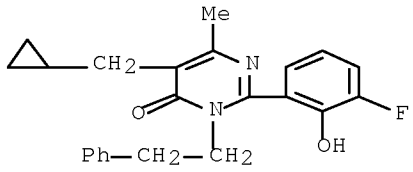
RN 938178-62-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(cyclobutylmethyl)-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



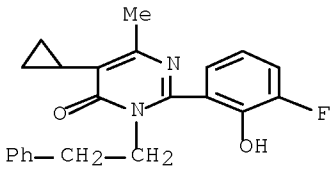
RN 938178-63-3 ZCAPLUS
CN 4(3H)-Quinazolinone, 5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)-6,6-dimethyl-3-(2-phenylethyl)- (CA INDEX NAME)



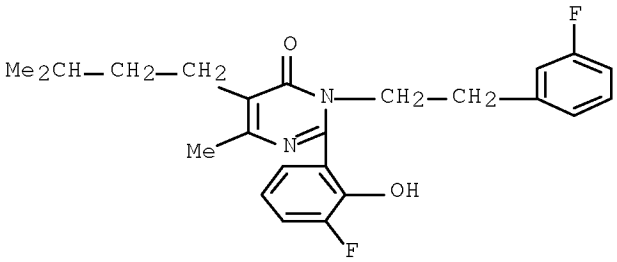
RN 938178-64-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(cyclopropylmethyl)-2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



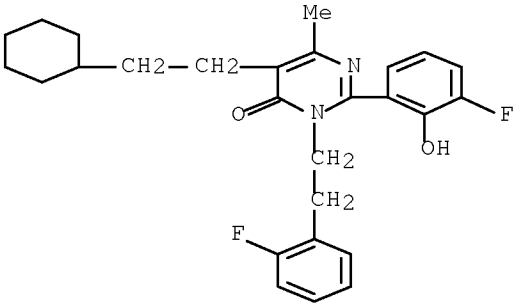
RN 938178-65-5 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-cyclopropyl-2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



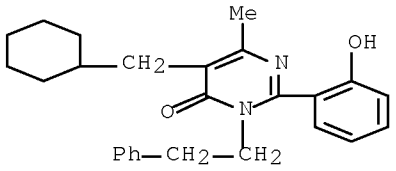
RN 938178-66-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl-5-(3-methylbutyl)- (CA INDEX NAME)



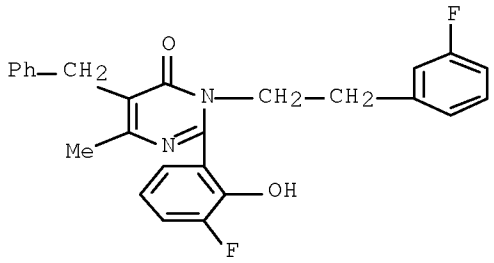
RN 938178-67-7 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(2-cyclohexylethyl)-2-(3-fluoro-2-hydroxyphenyl)-3-[2-(2-fluorophenyl)ethyl]-6-methyl- (CA INDEX NAME)



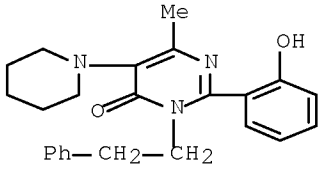
RN 938178-68-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(cyclohexylmethyl)-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



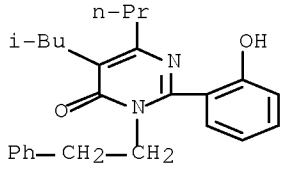
RN 938178-69-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl-5-(phenylmethyl)- (CA INDEX NAME)



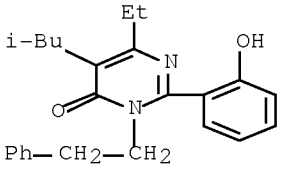
RN 938178-71-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)-5-(1-piperidinyl)- (CA INDEX NAME)



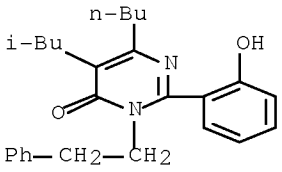
RN 938178-79-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-5-(2-methylpropyl)-3-(2-phenylethyl)-6-propyl- (CA INDEX NAME)



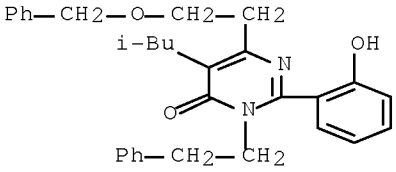
RN 938178-80-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 6-ethyl-2-(2-hydroxyphenyl)-5-(2-methylpropyl)-3-(2-phenylethyl)- (CA INDEX NAME)



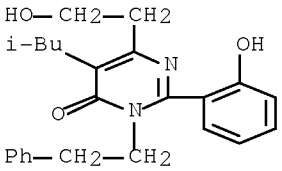
RN 938178-81-5 ZCAPLUS
CN 4(3H)-Pyrimidinone, 6-butyl-2-(2-hydroxyphenyl)-5-(2-methylpropyl)-3-(2-phenylethyl)- (CA INDEX NAME)



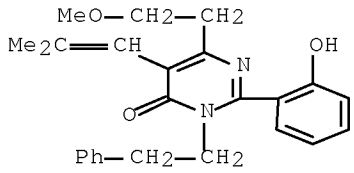
RN 938178-82-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-5-(2-methylpropyl)-3-(2-phenylethyl)-6-[2-(phenylmethoxy)ethyl]- (CA INDEX NAME)



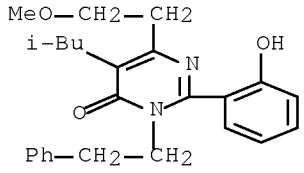
RN 938178-83-7 ZCAPLUS
CN 4(3H)-Pyrimidinone, 6-(2-hydroxyethyl)-2-(2-hydroxyphenyl)-5-(2-methylpropyl)-3-(2-phenylethyl)- (CA INDEX NAME)



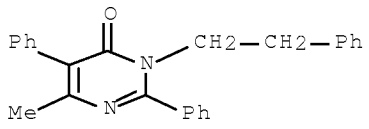
RN 938178-84-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-(2-methoxyethyl)-5-(2-methyl-1-propen-1-yl)-3-(2-phenylethyl)- (CA INDEX NAME)



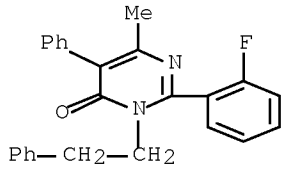
RN 938178-85-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-(2-methoxyethyl)-5-(2-methylpropyl)-3-(2-phenylethyl)- (CA INDEX NAME)



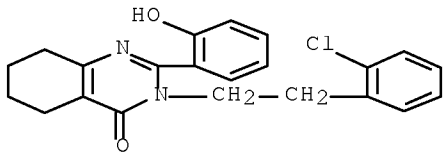
RN 938178-88-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 6-methyl-2,5-diphenyl-3-(2-phenylethyl)- (CA INDEX NAME)



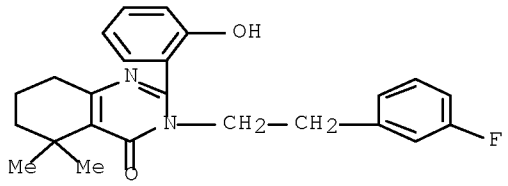
RN 938178-89-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-fluorophenyl)-6-methyl-5-phenyl-3-(2-phenylethyl)- (CA INDEX NAME)



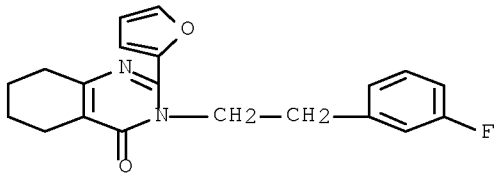
RN 938178-90-6 ZCAPLUS
CN 4(3H)-Quinazolinone, 3-[2-(2-chlorophenyl)ethyl]-5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)- (CA INDEX NAME)



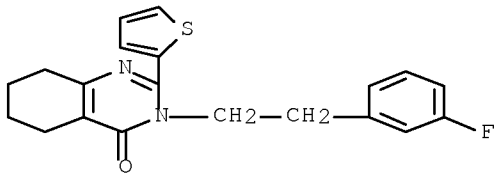
RN 938178-91-7 ZCAPLUS
CN 4(3H)-Quinazolinone, 3-[2-(3-fluorophenyl)ethyl]-5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)-5,5-dimethyl- (CA INDEX NAME)



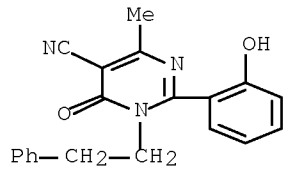
RN 938178-93-9 ZCAPLUS
CN 4(3H)-Quinazolinone, 3-[2-(3-fluorophenyl)ethyl]-2-(2-furanyl)-5,6,7,8-tetrahydro- (CA INDEX NAME)



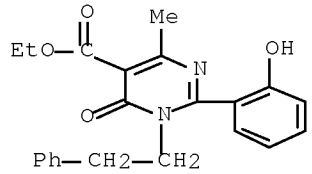
RN 938178-94-0 ZCAPLUS
CN 4(3H)-Quinazolinone, 3-[2-(3-fluorophenyl)ethyl]-5,6,7,8-tetrahydro-2-(2-thienyl)- (CA INDEX NAME)



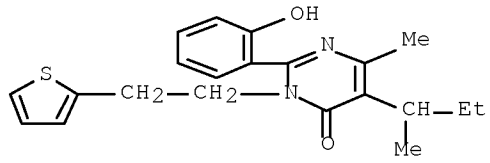
RN 938178-95-1 ZCAPLUS
CN 5-Pyrimidinecarbonitrile, 1,6-dihydro-2-(2-hydroxyphenyl)-4-methyl-6-oxo-1-(2-phenylethyl)- (CA INDEX NAME)



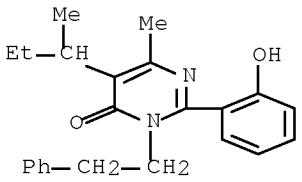
RN 938178-96-2 ZCAPLUS
CN 5-Pyrimidinecarboxylic acid, 1,6-dihydro-2-(2-hydroxyphenyl)-4-methyl-6-oxo-1-(2-phenylethyl)-, ethyl ester (CA INDEX NAME)



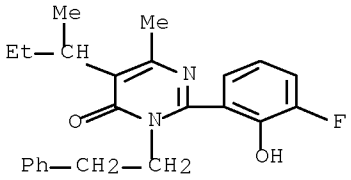
RN 938178-97-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-5-(1-methylpropyl)-3-[2-(2-thienyl)ethyl]- (CA INDEX NAME)



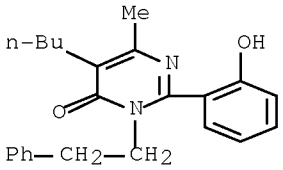
RN 938178-98-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-5-(1-methylpropyl)-3-(2-phenylethyl)- (CA INDEX NAME)



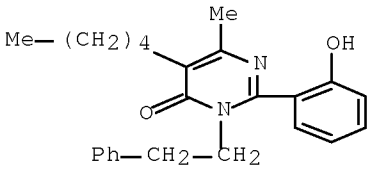
RN 938178-99-5 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-5-(1-methylpropyl)-3-(2-phenylethyl)- (CA INDEX NAME)



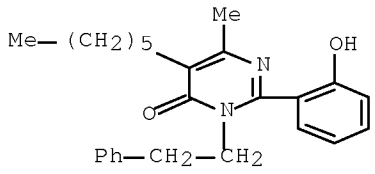
RN 938179-00-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-butyl-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



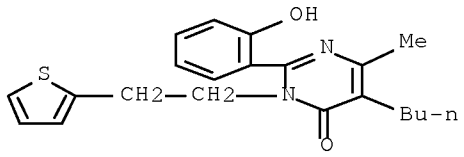
RN 938179-01-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-5-pentyl-3-(2-phenylethyl)- (CA INDEX NAME)



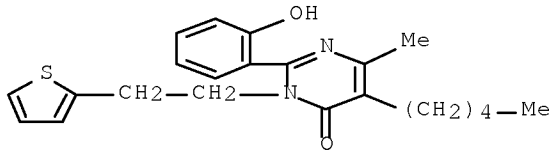
RN 938179-02-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-hexyl-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



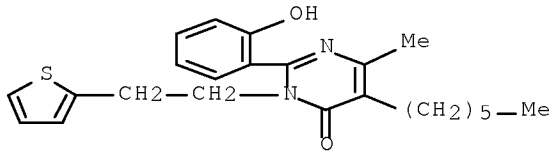
RN 938179-05-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-butyl-2-(2-hydroxyphenyl)-6-methyl-3-[2-(2-thienyl)ethyl]- (CA INDEX NAME)



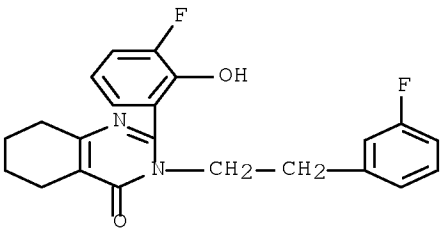
RN 938179-06-7 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-5-pentyl-3-[2-(2-thienyl)ethyl]- (CA INDEX NAME)



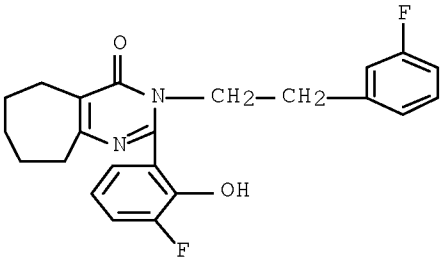
RN 938179-07-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-hexyl-2-(2-hydroxyphenyl)-6-methyl-3-[2-(2-thienyl)ethyl]- (CA INDEX NAME)



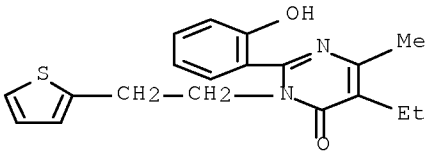
RN 938179-08-9 ZCAPLUS
CN 4(3H)-Quinazolinone, 2-(3-fluoro-2-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-5,6,7,8-tetrahydro- (CA INDEX NAME)



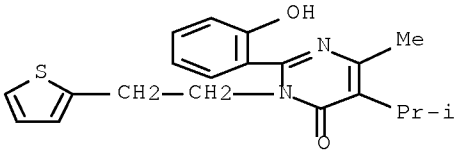
RN 938179-09-0 ZCAPLUS
CN 4H-Cycloheptapyrimidin-4-one, 2-(3-fluoro-2-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-3,5,6,7,8,9-hexahydro- (CA INDEX NAME)



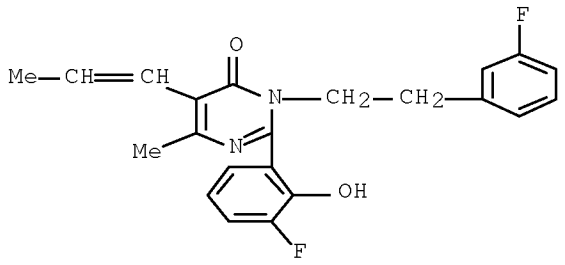
RN 938179-12-5 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-2-(2-hydroxyphenyl)-6-methyl-3-[2-(2-thienyl)ethyl]- (CA INDEX NAME)



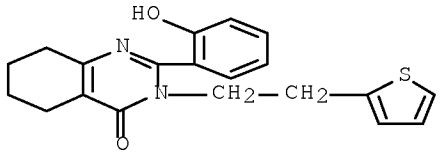
RN 938179-13-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-5-(1-methylethyl)-3-[2-(2-thienyl)ethyl]- (CA INDEX NAME)



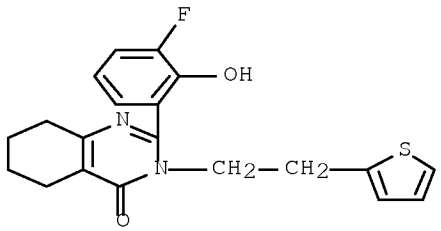
RN 938179-16-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl-5-(1-propen-1-yl)- (CA INDEX NAME)



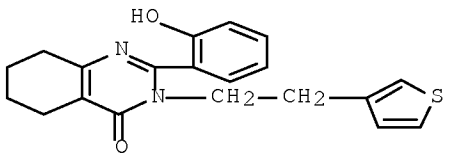
RN 938179-18-1 ZCAPLUS
CN 4(3H)-Quinazolinone, 5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)-3-[2-(2-thienyl)ethyl]- (CA INDEX NAME)



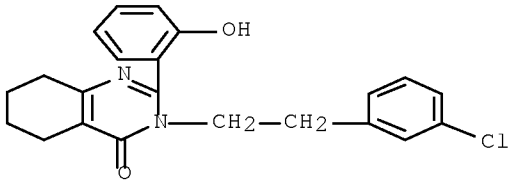
RN 938179-19-2 ZCAPLUS
CN 4(3H)-Quinazolinone, 2-(3-fluoro-2-hydroxyphenyl)-5,6,7,8-tetrahydro-3-[2-(2-thienyl)ethyl]- (CA INDEX NAME)



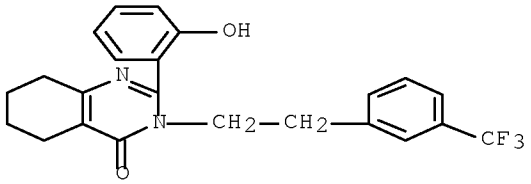
RN 938179-20-5 ZCAPLUS
CN 4(3H)-Quinazolinone, 5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)-3-[2-(3-thienyl)ethyl]- (CA INDEX NAME)



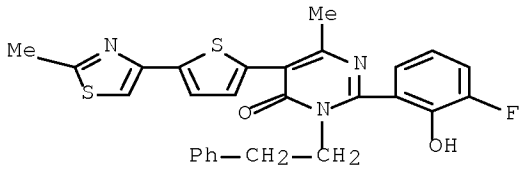
RN 938179-21-6 ZCAPLUS
CN 4(3H)-Quinazolinone, 3-[2-(3-chlorophenyl)ethyl]-5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)- (CA INDEX NAME)



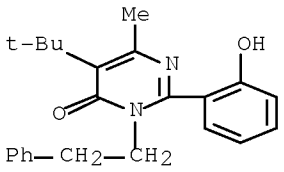
RN 938179-23-8 ZCAPLUS
CN 4(3H)-Quinazolinone, 5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)-3-[2-[3-(trifluoromethyl)phenyl]ethyl]- (CA INDEX NAME)



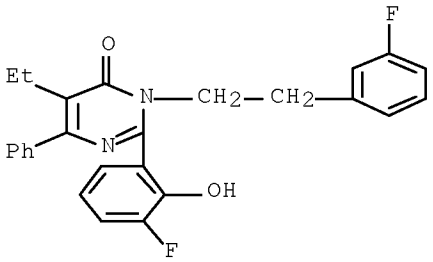
RN 938179-28-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-5-[5-(2-methyl-4-thiazolyl)-2-thienyl]-3-(2-phenylethyl)- (CA INDEX NAME)



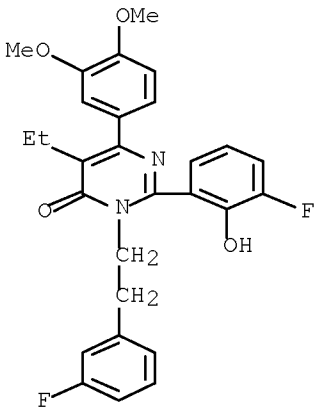
RN 938179-33-0 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(1,1-dimethylethyl)-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



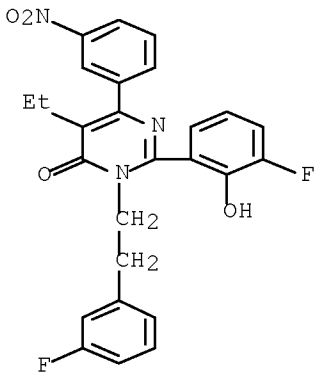
RN 938179-35-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-2-(3-fluoro-2-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-phenyl- (CA INDEX NAME)



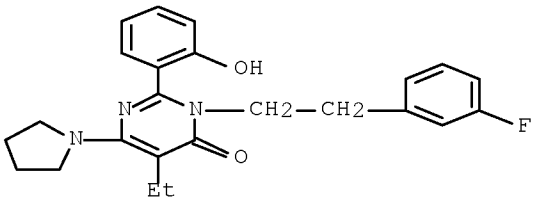
RN 938179-36-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 6-(3,4-dimethoxyphenyl)-5-ethyl-2-(3-fluoro-2-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]- (CA INDEX NAME)



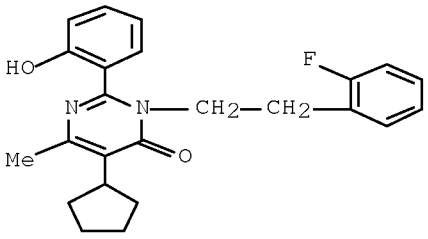
RN 938179-37-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-2-(3-fluoro-2-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-(3-nitrophenyl)- (CA INDEX NAME)



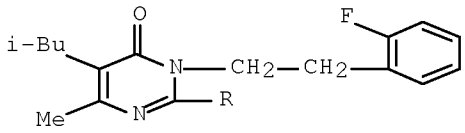
RN 938179-38-5 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-3-[2-(3-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-(1-pyrrolidinyl)- (CA INDEX NAME)

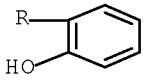


RN 938179-41-0 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-cyclopentyl-3-[2-(2-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl- (CA INDEX NAME)

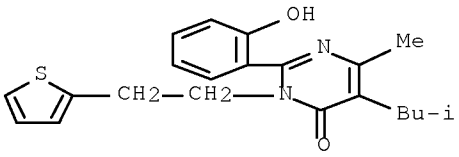


RN 938179-42-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-[2-(2-fluorophenyl)ethyl]-2-(2-hydroxyphenyl)-6-methyl-5-(2-methylpropyl)- (CA INDEX NAME)

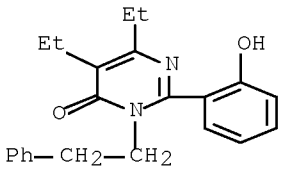




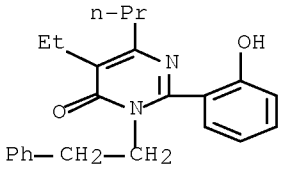
RN 938179-43-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-5-(2-methylpropyl)-3-[2-(2-thienyl)ethyl]- (CA INDEX NAME)



RN 938179-44-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5,6-diethyl-2-(2-hydroxyphenyl)-3-(2-phenylethyl)- (CA INDEX NAME)

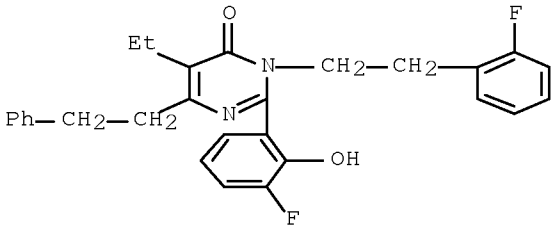


RN 938179-45-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-2-(2-hydroxyphenyl)-3-(2-phenylethyl)-6-propyl- (CA INDEX NAME)



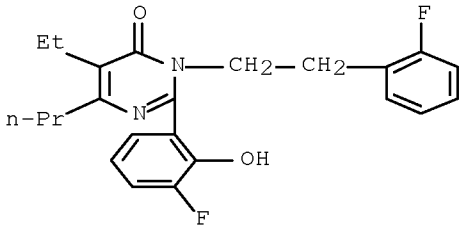
RN 938179-46-5 ZCAPLUS

CN 4(3H)-Pyrimidinone, 5-ethyl-2-(3-fluoro-2-hydroxyphenyl)-3-[2-(2-fluorophenyl)ethyl]-6-(2-phenylethyl)- (CA INDEX NAME)



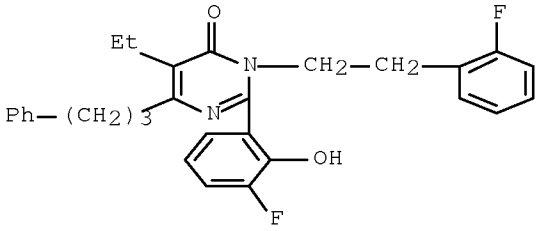
RN 938179-47-6 ZCAPLUS

CN 4(3H)-Pyrimidinone, 5-ethyl-2-(3-fluoro-2-hydroxyphenyl)-3-[2-(2-fluorophenyl)ethyl]-6-propyl- (CA INDEX NAME)



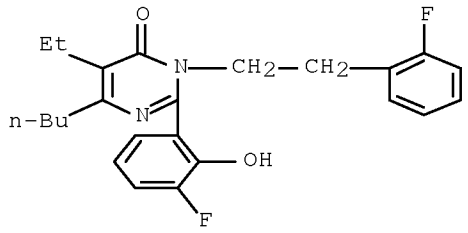
RN 938179-48-7 ZCAPLUS

CN 4(3H)-Pyrimidinone, 5-ethyl-2-(3-fluoro-2-hydroxyphenyl)-3-[2-(2-fluorophenyl)ethyl]-6-(3-phenylpropyl)- (CA INDEX NAME)

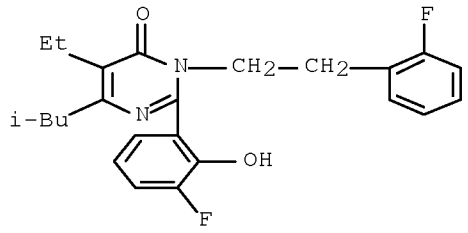


RN 938179-49-8 ZCAPLUS

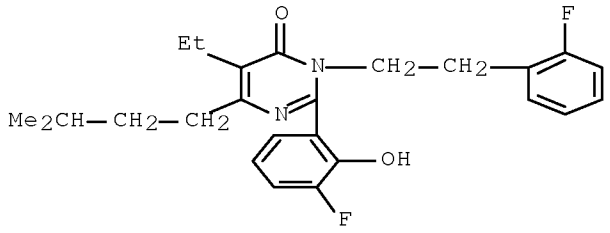
CN 4(3H)-Pyrimidinone, 6-butyl-5-ethyl-2-(3-fluoro-2-hydroxyphenyl)-3-[2-(2-fluorophenyl)ethyl]- (CA INDEX NAME)



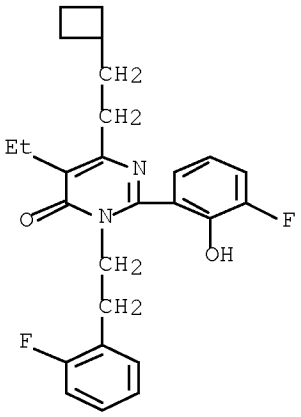
RN 938179-50-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-2-(3-fluoro-2-hydroxyphenyl)-3-[2-(2-fluorophenyl)ethyl]-6-(2-methylpropyl)- (CA INDEX NAME)



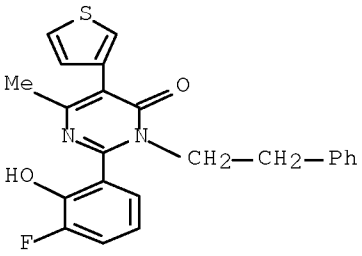
RN 938179-51-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-2-(3-fluoro-2-hydroxyphenyl)-3-[2-(2-fluorophenyl)ethyl]-6-(3-methylbutyl)- (CA INDEX NAME)



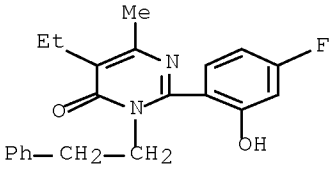
RN 938179-52-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 6-(2-cyclobutylethyl)-5-ethyl-2-(3-fluoro-2-hydroxyphenyl)-3-[2-(2-fluorophenyl)ethyl]- (CA INDEX NAME)



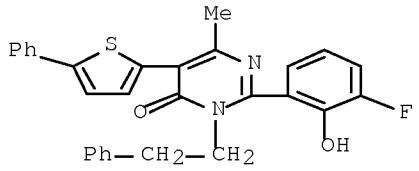
RN 938179-53-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)-5-(3-thienyl)- (CA INDEX NAME)



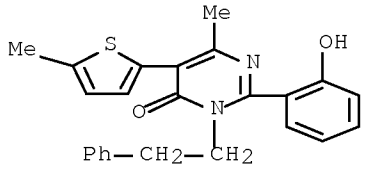
RN 938179-54-5 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-2-(4-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



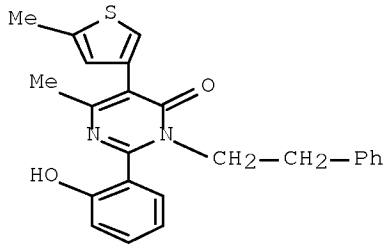
RN 938179-55-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)-5-(5-phenyl-2-thienyl)- (CA INDEX NAME)



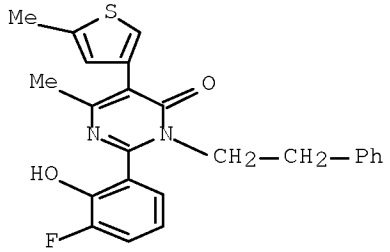
RN 938179-56-7 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-5-(5-methyl-2-thienyl)-3-(2-phenylethyl)- (CA INDEX NAME)



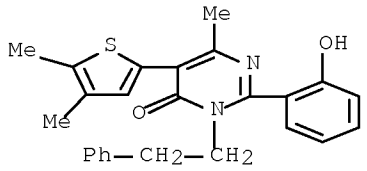
RN 938179-57-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-5-(5-methyl-3-thienyl)-3-(2-phenylethyl)- (CA INDEX NAME)



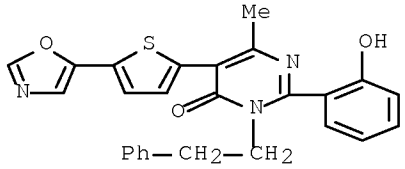
RN 938179-58-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-5-(5-methyl-3-thienyl)-3-(2-phenylethyl)- (CA INDEX NAME)



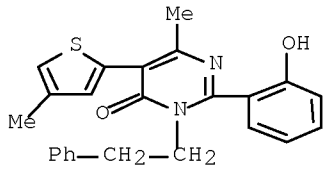
RN 938179-59-0 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(4,5-dimethyl-2-thienyl)-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



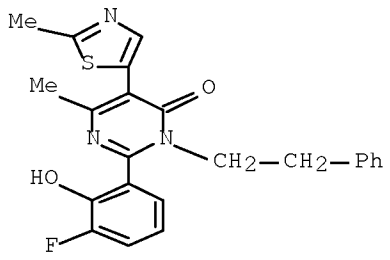
RN 938179-60-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-5-[5-(5-oxazolyl)-2-thienyl]-3-(2-phenylethyl)- (CA INDEX NAME)



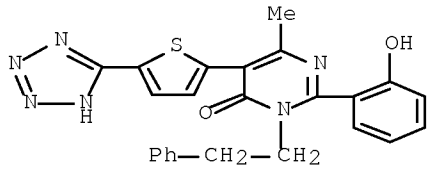
RN 938179-61-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-5-(4-methyl-2-thienyl)-3-(2-phenylethyl)- (CA INDEX NAME)



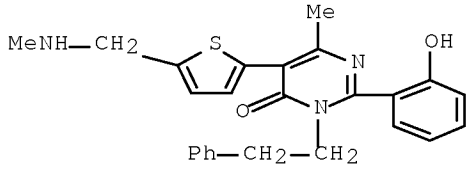
RN 938179-62-5 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-5-(2-methyl-5-thiazolyl)-3-(2-phenylethyl)- (CA INDEX NAME)



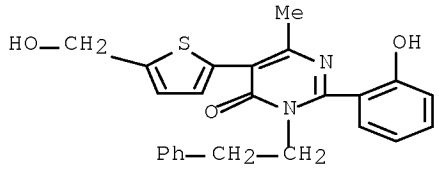
RN 938179-63-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)-5-[5-(2H-tetrazol-5-yl)-2-thienyl]- (CA INDEX NAME)



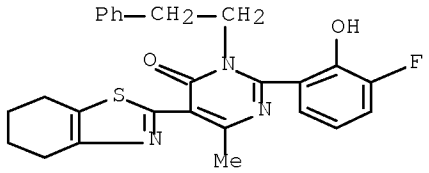
RN 938179-65-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-5-[5-[(methylamino)methyl]-2-thienyl]-3-(2-phenylethyl)- (CA INDEX NAME)



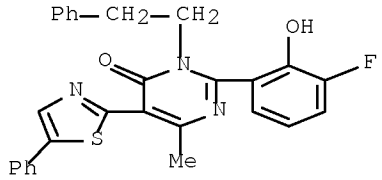
RN 938179-66-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-[5-(hydroxymethyl)-2-thienyl]-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



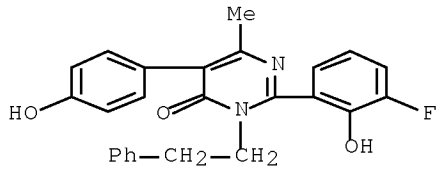
RN 938179-67-0 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)-5-(4,5,6,7-tetrahydro-2-benzothiazolyl)- (CA INDEX NAME)



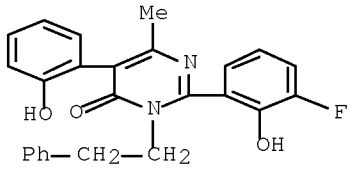
RN 938179-68-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)-5-(5-phenyl-2-thiazolyl)- (CA INDEX NAME)



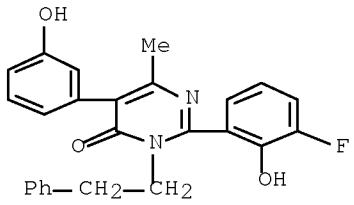
RN 938179-69-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-5-(4-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



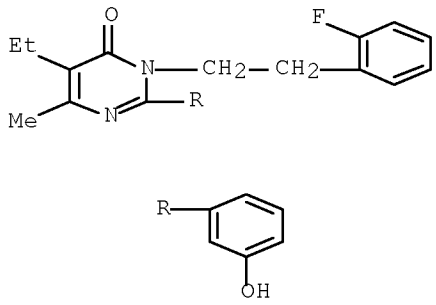
RN 938179-70-5 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-5-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



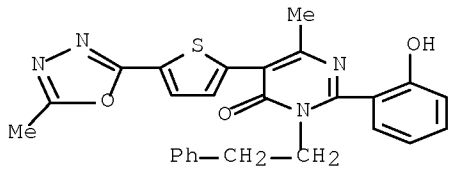
RN 938179-71-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-5-(3-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



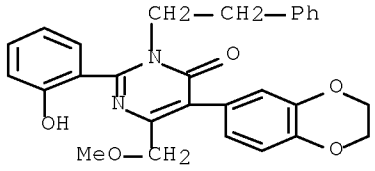
RN 938179-73-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-3-[2-(2-fluorophenyl)ethyl]-2-(3-hydroxyphenyl)-6-methyl- (CA INDEX NAME)



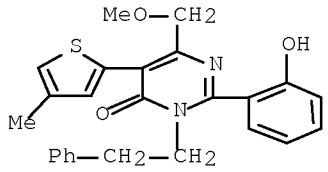
RN 938179-74-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-5-[5-(5-methyl-1,3,4-oxadiazol-2-yl)-2-thienyl]-3-(2-phenylethyl)- (CA INDEX NAME)



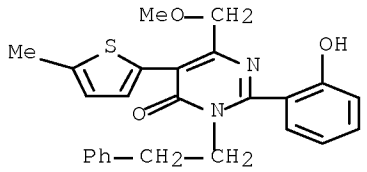
RN 938179-75-0 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-(2-hydroxyphenyl)-6-(methoxymethyl)-3-(2-phenylethyl)- (CA INDEX NAME)



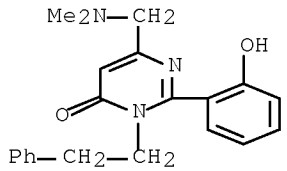
RN 938179-76-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-(methoxymethyl)-5-(4-methyl-2-thienyl)-3-(2-phenylethyl)- (CA INDEX NAME)



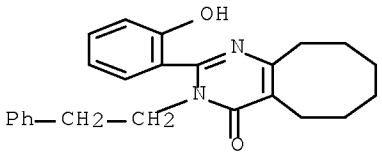
RN 938179-77-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-(methoxymethyl)-5-(5-methyl-2-thienyl)-3-(2-phenylethyl)- (CA INDEX NAME)



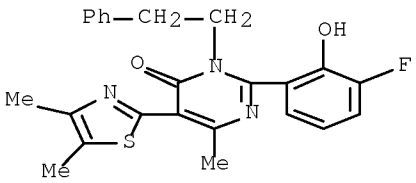
RN 938179-79-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 6-[(dimethylamino)methyl]-2-(2-hydroxyphenyl)-3-(2-phenylethyl)- (CA INDEX NAME)



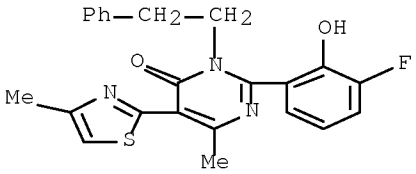
RN 938179-80-7 ZCAPLUS
CN 4(3H)-Cyclooctapyrimidinone, 5,6,7,8,9,10-hexahydro-2-(2-hydroxyphenyl)-3-(2-phenylethyl)- (CA INDEX NAME)



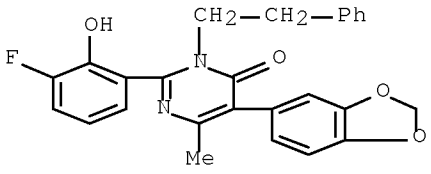
RN 938179-81-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(4,5-dimethyl-2-thiazolyl)-2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



RN 938179-82-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-5-(4-methyl-2-thiazolyl)-3-(2-phenylethyl)- (CA INDEX NAME)

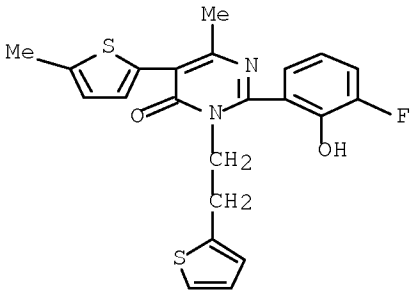


RN 938179-83-0 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(1,3-benzodioxol-5-yl)-2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)

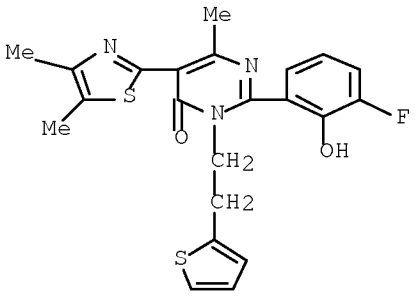


RN 938179-90-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-5-(5-methyl-2-

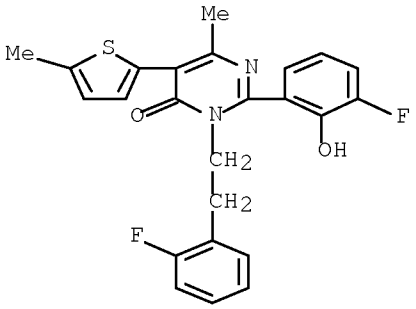
thienyl)-3-[2-(2-thienyl)ethyl]- (CA INDEX NAME)



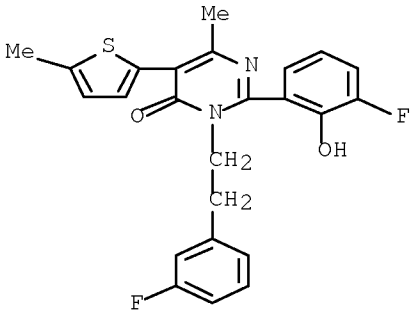
RN 938179-91-0 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(4,5-dimethyl-2-thiazolyl)-2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-[2-(2-thienyl)ethyl]- (CA INDEX NAME)



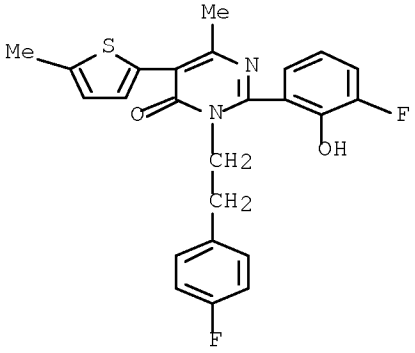
RN 938179-93-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-3-[2-(2-fluorophenyl)ethyl]-6-methyl-5-(5-methyl-2-thienyl)- (CA INDEX NAME)



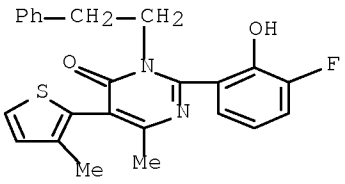
RN 938179-94-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-3-[2-(3-fluorophenyl)ethyl]-6-methyl-5-(5-methyl-2-thienyl)- (CA INDEX NAME)



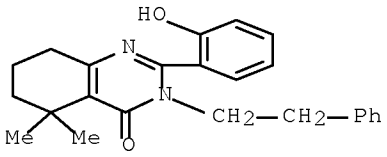
RN 938179-95-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-3-[2-(4-fluorophenyl)ethyl]-6-methyl-5-(5-methyl-2-thienyl)- (CA INDEX NAME)



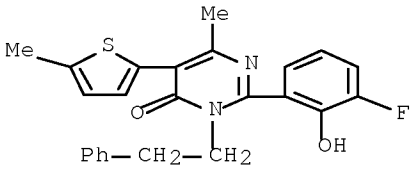
RN 938179-96-5 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-5-(3-methyl-2-thienyl)-3-(2-phenylethyl)- (CA INDEX NAME)



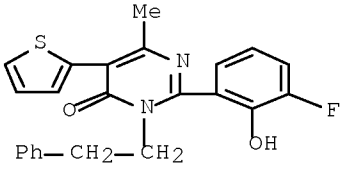
RN 938179-99-8 ZCAPLUS
CN 4(3H)-Quinazolinone, 5,6,7,8-tetrahydro-2-(2-hydroxyphenyl)-5,5-dimethyl-3-(2-phenylethyl)- (CA INDEX NAME)



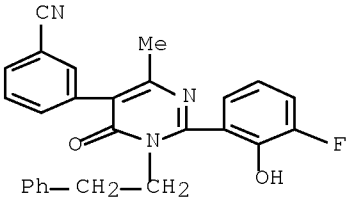
RN 938180-01-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-5-(5-methyl-2-thienyl)-3-(2-phenylethyl)- (CA INDEX NAME)



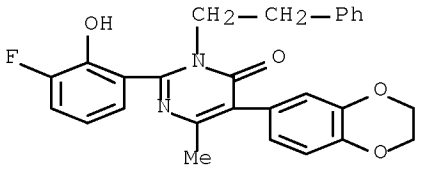
RN 938180-02-0 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)-5-(2-thienyl)- (CA INDEX NAME)



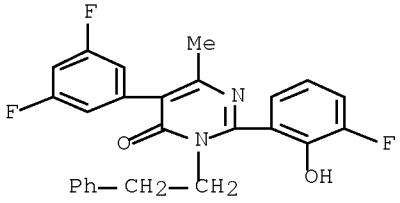
RN 938180-03-1 ZCAPLUS
CN Benzonitrile, 3-[2-(3-fluoro-2-hydroxyphenyl)-1,6-dihydro-4-methyl-6-oxo-1-(2-phenylethyl)-5-pyrimidinyl]- (CA INDEX NAME)



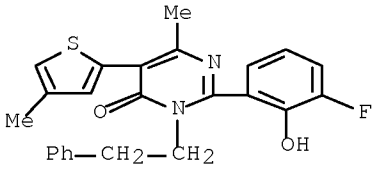
RN 938180-04-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(2,3-dihydro-1,4-benzodioxin-6-yl)-2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



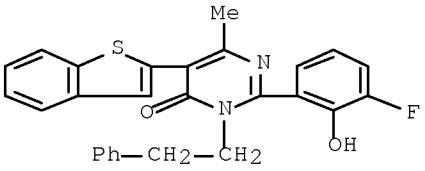
RN 938180-05-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(3,5-difluorophenyl)-2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



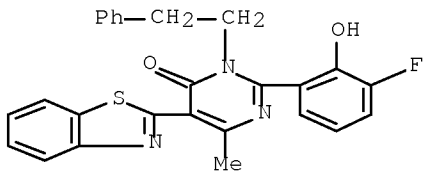
RN 938180-06-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-5-(4-methyl-2-thienyl)-3-(2-phenylethyl)- (CA INDEX NAME)



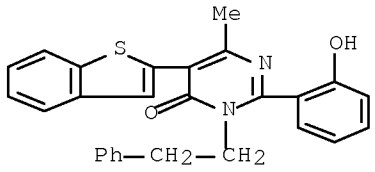
RN 938180-07-5 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-benzo[b]thien-2-yl-2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



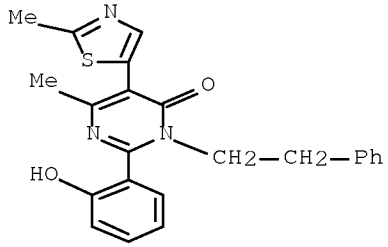
RN 938180-08-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(2-benzothiazolyl)-2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



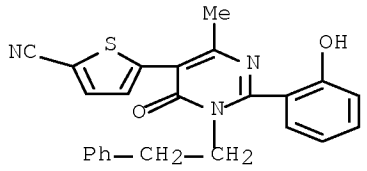
RN 938180-09-7 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-benzo[b]thien-2-yl-2-(2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



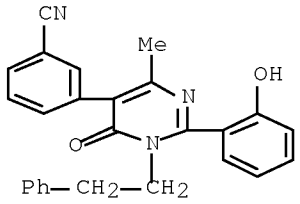
RN 938180-10-0 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-hydroxyphenyl)-6-methyl-5-(2-methyl-5-thiazolyl)-3-(2-phenylethyl)- (CA INDEX NAME)



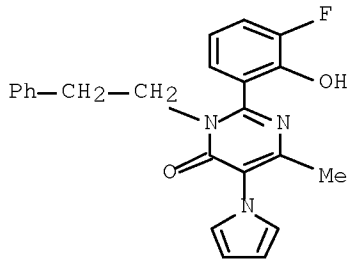
RN 938180-11-1 ZCAPLUS
CN 2-Thiophenecarbonitrile, 5-[1,6-dihydro-2-(2-hydroxyphenyl)-4-methyl-6-oxo-1-(2-phenylethyl)-5-pyrimidinyl]- (CA INDEX NAME)



RN 938180-12-2 ZCAPLUS
CN Benzonitrile, 3-[1,6-dihydro-2-(2-hydroxyphenyl)-4-methyl-6-oxo-1-(2-phenylethyl)-5-pyrimidinyl]- (CA INDEX NAME)



RN 938180-15-5 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)-5-(1H-pyrrol-1-yl)- (CA INDEX NAME)



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938180-31-5P 938180-33-7P 938180-39-3P
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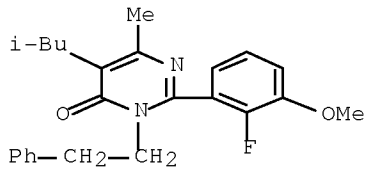
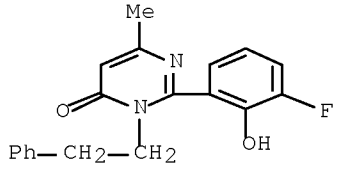
938181-72-7P 938181-77-2P 938181-78-3P
938181-79-4P 938181-80-7P 938181-81-8P
938181-82-9P 938181-93-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)

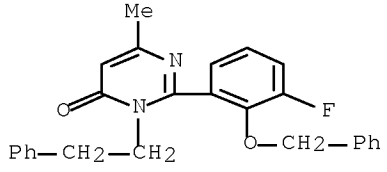
RN 938180-17-7 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-fluoro-3-methoxyphenyl)-6-methyl-5-(2-methylpropyl)-3-(2-phenylethyl)- (CA INDEX NAME)



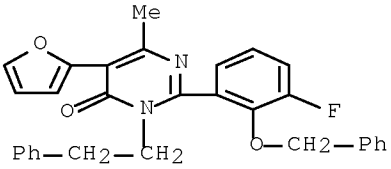
RN 938180-20-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



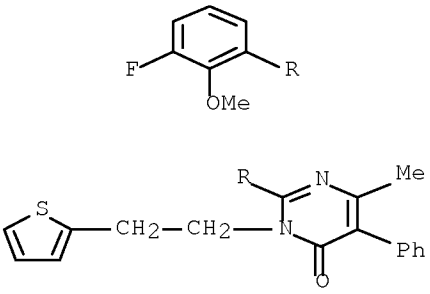
RN 938180-21-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-[3-fluoro-2-(phenylmethoxy)phenyl]-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



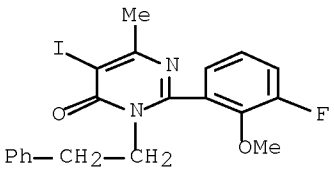
RN 938180-23-5 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-[3-fluoro-2-(phenylmethoxy)phenyl]-5-(2-furanyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



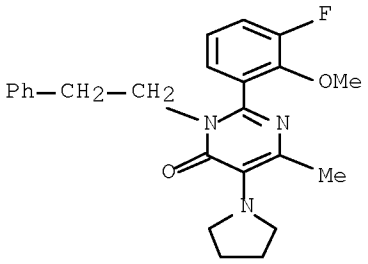
RN 938180-26-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-methoxyphenyl)-6-methyl-5-phenyl-3-[2-(2-thienyl)ethyl]- (CA INDEX NAME)



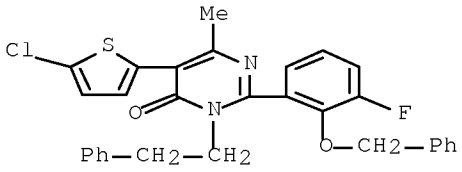
RN 938180-27-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-methoxyphenyl)-5-iodo-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



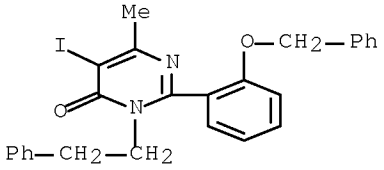
RN 938180-28-0 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-methoxyphenyl)-6-methyl-3-(2-phenylethyl)-5-(1-pyrrolidinyl)- (CA INDEX NAME)



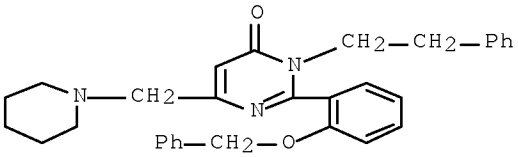
RN 938180-29-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(5-chloro-2-thienyl)-2-[3-fluoro-2-(phenylmethoxy)phenyl]-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



RN 938180-30-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-iodo-6-methyl-3-(2-phenylethyl)-2-[2-(phenylmethoxy)phenyl]- (CA INDEX NAME)

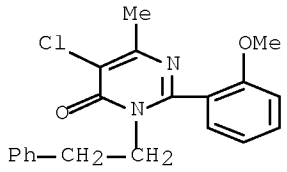


RN 938180-31-5 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-(2-phenylethyl)-2-[2-(phenylmethoxy)phenyl]-6-(1-piperidinylmethyl)- (CA INDEX NAME)



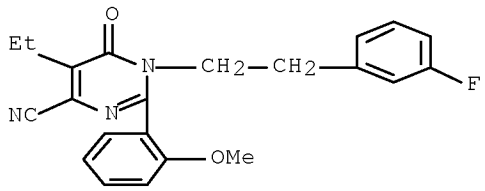
RN 938180-33-7 ZCAPLUS

CN 4(3H)-Pyrimidinone, 5-chloro-2-(2-methoxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



RN 938180-39-3 ZCAPLUS

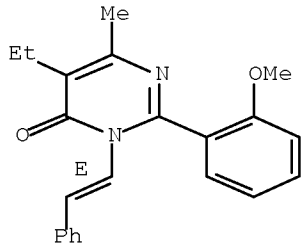
CN 4-Pyrimidinecarbonitrile, 5-ethyl-1-[2-(3-fluorophenyl)ethyl]-1,6-dihydro-2-(2-methoxyphenyl)-6-oxo- (CA INDEX NAME)



RN 938180-40-6 ZCAPLUS

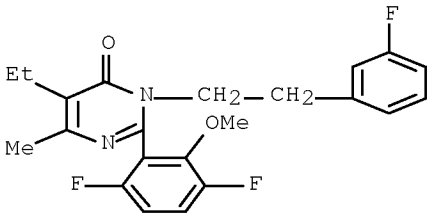
CN 4(3H)-Pyrimidinone, 5-ethyl-2-(2-methoxyphenyl)-6-methyl-3-[(1E)-2-phenylethenyl]- (CA INDEX NAME)

Double bond geometry as shown.

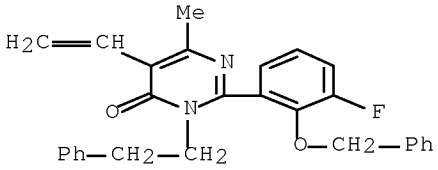


RN 938180-43-9 ZCAPLUS

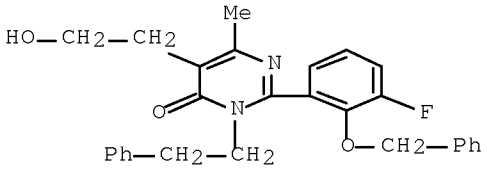
CN 4(3H)-Pyrimidinone, 2-(3,6-difluoro-2-methoxyphenyl)-5-ethyl-3-[2-(3-fluorophenyl)ethyl]-6-methyl- (CA INDEX NAME)



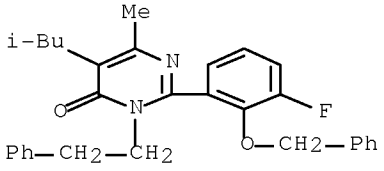
RN 938180-46-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-ethenyl-2-[3-fluoro-2-(phenylmethoxy)phenyl]-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



RN 938180-47-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-[3-fluoro-2-(phenylmethoxy)phenyl]-5-(2-hydroxyethyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)

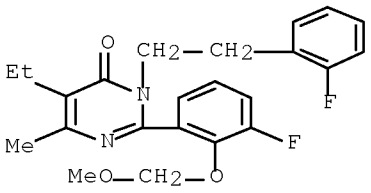


RN 938180-53-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-[3-fluoro-2-(phenylmethoxy)phenyl]-6-methyl-5-(2-methylpropyl)-3-(2-phenylethyl)- (CA INDEX NAME)

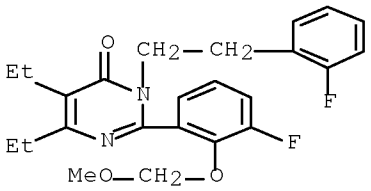


RN 938180-55-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-2-[3-fluoro-2-(methoxymethoxy)phenyl]-3-[2-(2-

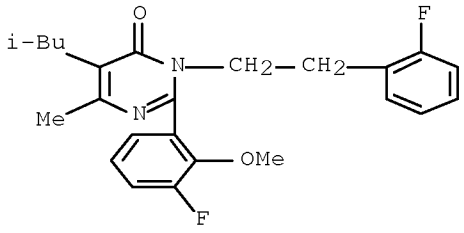
fluorophenyl)ethyl]-6-methyl- (CA INDEX NAME)



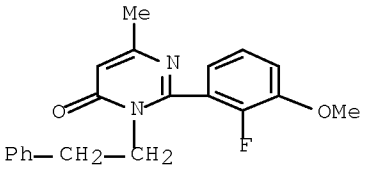
RN 938180-56-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5,6-diethyl-2-[3-fluoro-2-(methoxymethoxy)phenyl]-3-[2-(2-fluorophenyl)ethyl]- (CA INDEX NAME)



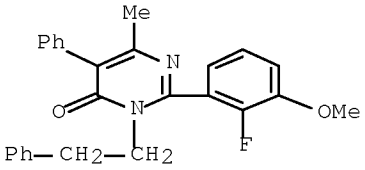
RN 938180-58-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-methoxyphenyl)-3-[2-(2-fluorophenyl)ethyl]-6-methyl-5-(2-methylpropyl)- (CA INDEX NAME)



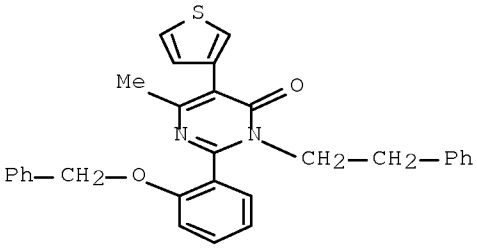
RN 938180-65-5 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-fluoro-3-methoxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



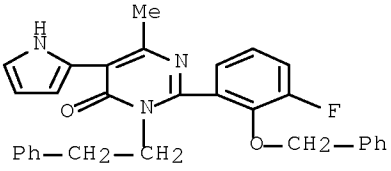
RN 938180-66-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(2-fluoro-3-methoxyphenyl)-6-methyl-5-phenyl-3-(2-phenylethyl)- (CA INDEX NAME)



RN 938180-67-7 ZCAPLUS
CN 4(3H)-Pyrimidinone, 6-methyl-3-(2-phenylethyl)-2-[2-(phenylmethoxy)phenyl]-5-(3-thienyl)- (CA INDEX NAME)

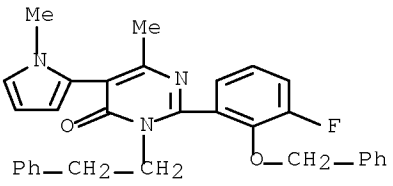


RN 938180-68-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-[3-fluoro-2-(phenylmethoxy)phenyl]-6-methyl-3-(2-phenylethyl)-5-(1H-pyrrol-2-yl)- (CA INDEX NAME)



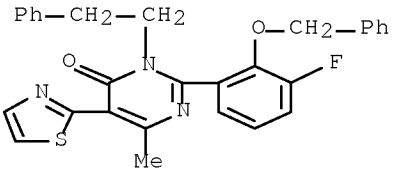
RN 938180-69-9 ZCAPLUS

CN 4(3H)-Pyrimidinone, 2-[3-fluoro-2-(phenylmethoxy)phenyl]-6-methyl-5-(1-methyl-1H-pyrrol-2-yl)-3-(2-phenylethyl)- (CA INDEX NAME)



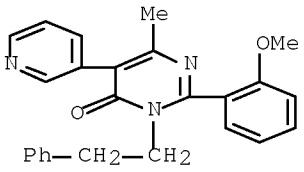
RN 938180-70-2 ZCAPLUS

CN 4(3H)-Pyrimidinone, 2-[3-fluoro-2-(phenylmethoxy)phenyl]-6-methyl-3-(2-phenylethyl)-5-(2-thiazolyl)- (CA INDEX NAME)



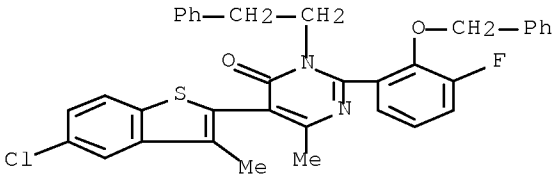
RN 938180-71-3 ZCAPLUS

CN 4(3H)-Pyrimidinone, 2-(2-methoxyphenyl)-6-methyl-3-(2-phenylethyl)-5-(3-pyridinyl)- (CA INDEX NAME)

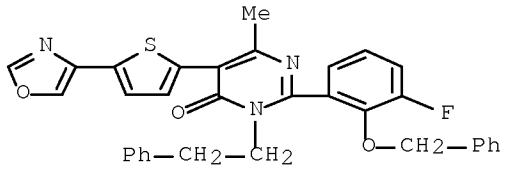


RN 938180-72-4 ZCAPLUS

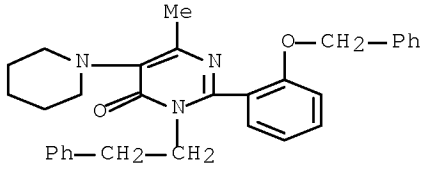
CN 4(3H)-Pyrimidinone, 5-(5-chloro-3-methylbenzo[b]thien-2-yl)-2-[3-fluoro-2-(phenylmethoxy)phenyl]-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



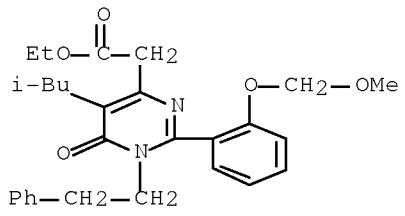
RN 938180-74-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-[3-fluoro-2-(phenylmethoxy)phenyl]-6-methyl-5-[5-(4-oxazolyl)-2-thienyl]-3-(2-phenylethyl)- (CA INDEX NAME)



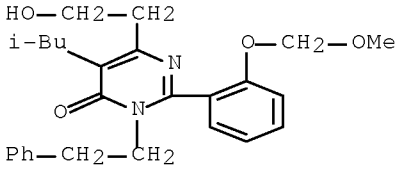
RN 938180-83-7 ZCAPLUS
CN 4(3H)-Pyrimidinone, 6-methyl-3-(2-phenylethyl)-2-[2-(phenylmethoxy)phenyl]-5-(1-piperidinyl)- (CA INDEX NAME)



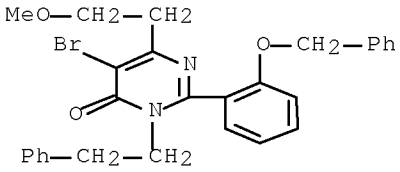
RN 938180-91-7 ZCAPLUS
CN 4-Pyrimidineacetic acid, 1,6-dihydro-2-[2-(methoxymethoxy)phenyl]-5-(2-methylpropyl)-6-oxo-1-(2-phenylethyl)-, ethyl ester (CA INDEX NAME)



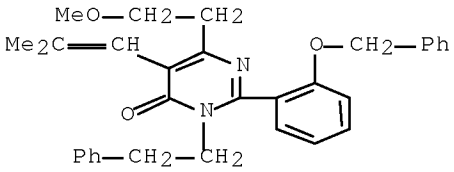
RN 938180-92-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 6-(2-hydroxyethyl)-2-[2-(methoxymethoxy)phenyl]-5-(2-methylpropyl)-3-(2-phenylethyl)- (CA INDEX NAME)



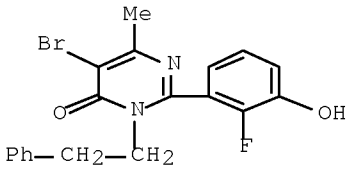
RN 938180-93-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-bromo-6-(2-methoxyethyl)-3-(2-phenylethyl)-2-[2-(phenylmethoxy)phenyl]- (CA INDEX NAME)



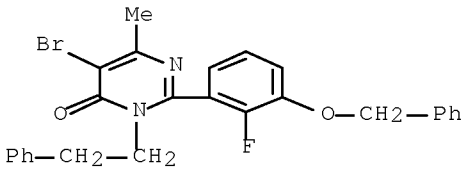
RN 938180-94-0 ZCAPLUS
CN 4(3H)-Pyrimidinone, 6-(2-methoxyethyl)-5-(2-methyl-1-propen-1-yl)-3-(2-phenylethyl)-2-[2-(phenylmethoxy)phenyl]- (CA INDEX NAME)



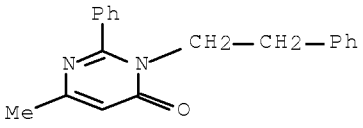
RN 938180-95-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-bromo-2-(2-fluoro-3-hydroxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



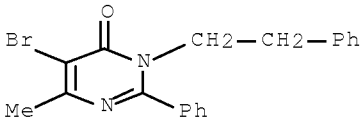
RN 938180-96-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-bromo-2-[2-fluoro-3-(phenylmethoxy)phenyl]-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



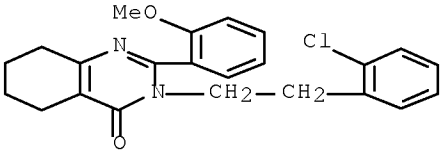
RN 938181-00-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 6-methyl-2-phenyl-3-(2-phenylethyl)- (CA INDEX NAME)



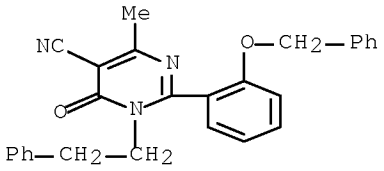
RN 938181-01-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-bromo-6-methyl-2-phenyl-3-(2-phenylethyl)- (CA INDEX NAME)



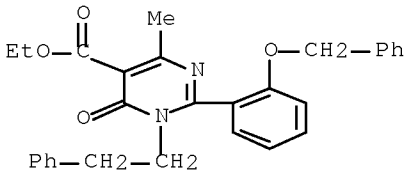
RN 938181-03-4 ZCAPLUS
CN 4(3H)-Quinazolinone, 3-[2-(2-chlorophenyl)ethyl]-5,6,7,8-tetrahydro-2-(2-methoxyphenyl)- (CA INDEX NAME)



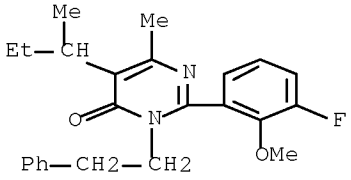
RN 938181-12-5 ZCAPLUS
CN 5-Pyrimidinecarbonitrile, 1,6-dihydro-4-methyl-6-oxo-1-(2-phenylethyl)-2-[2-(phenylmethoxy)phenyl]- (CA INDEX NAME)



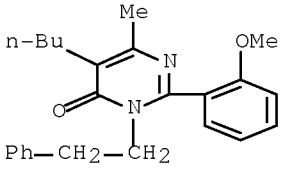
RN 938181-14-7 ZCAPLUS
CN 5-Pyrimidinecarboxylic acid, 1,6-dihydro-4-methyl-6-oxo-1-(2-phenylethyl)-2-[2-(phenylmethoxy)phenyl]-, ethyl ester (CA INDEX NAME)



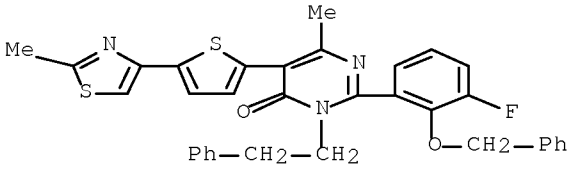
RN 938181-16-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-(3-fluoro-2-methoxyphenyl)-6-methyl-5-(1-methylpropyl)-3-(2-phenylethyl)- (CA INDEX NAME)



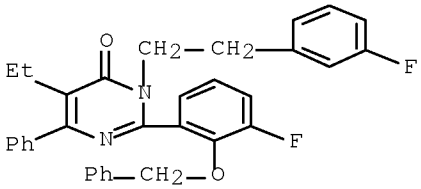
RN 938181-18-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-butyl-2-(2-methoxyphenyl)-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)



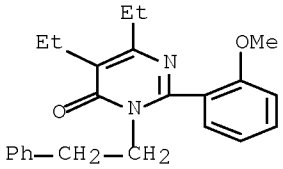
RN 938181-35-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-[3-fluoro-2-(phenylmethoxy)phenyl]-6-methyl-5-[5-(2-methyl-4-thiazolyl)-2-thienyl]-3-(2-phenylethyl)- (CA INDEX NAME)



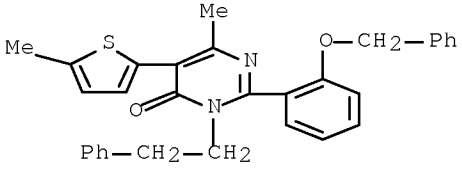
RN 938181-43-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-ethyl-3-[2-(3-fluorophenyl)ethyl]-2-[3-fluoro-2-(phenylmethoxy)phenyl]-6-phenyl- (CA INDEX NAME)



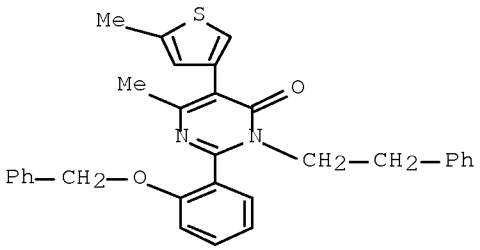
RN 938181-44-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5,6-diethyl-2-(2-methoxyphenyl)-3-(2-phenylethyl)- (CA INDEX NAME)



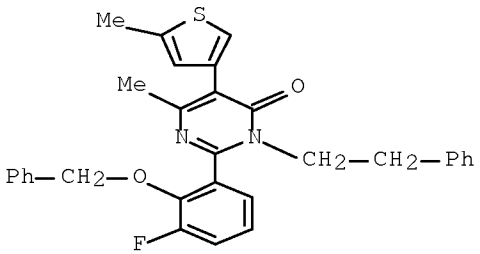
RN 938181-45-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 6-methyl-5-(5-methyl-2-thienyl)-3-(2-phenylethyl)-2-[2-(phenylmethoxy)phenyl]- (CA INDEX NAME)



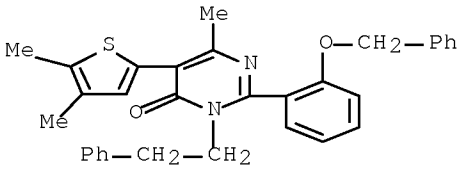
RN 938181-47-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 6-methyl-5-(5-methyl-3-thienyl)-3-(2-phenylethyl)-2-[2-(phenylmethoxy)phenyl]- (CA INDEX NAME)



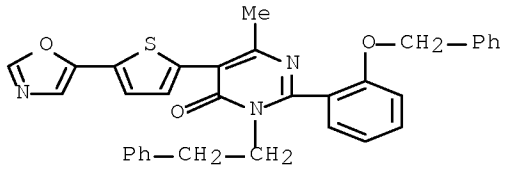
RN 938181-48-7 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-[3-fluoro-2-(phenylmethoxy)phenyl]-6-methyl-5-(5-methyl-3-thienyl)-3-(2-phenylethyl)- (CA INDEX NAME)



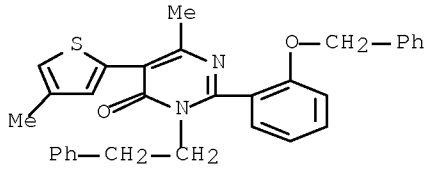
RN 938181-49-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(4,5-dimethyl-2-thienyl)-6-methyl-3-(2-phenylethyl)-2-[2-(phenylmethoxy)phenyl]- (CA INDEX NAME)



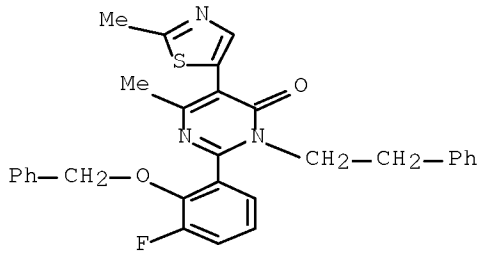
RN 938181-50-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 6-methyl-5-[5-(5-oxazolyl)-2-thienyl]-3-(2-phenylethyl)-2-[2-(phenylmethoxy)phenyl]- (CA INDEX NAME)



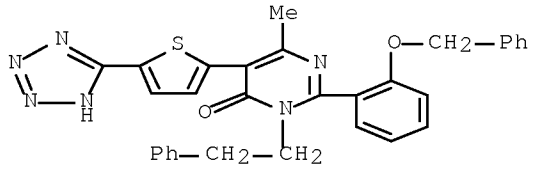
RN 938181-51-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 6-methyl-5-(4-methyl-2-thienyl)-3-(2-phenylethyl)-2-[2-(phenylmethoxy)phenyl]- (CA INDEX NAME)



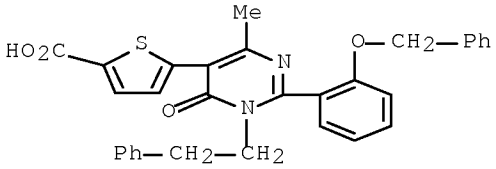
RN 938181-52-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-[3-fluoro-2-(phenylmethoxy)phenyl]-6-methyl-5-(2-methyl-5-thiazolyl)-3-(2-phenylethyl)- (CA INDEX NAME)



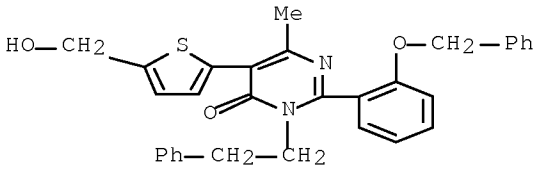
RN 938181-53-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 6-methyl-3-(2-phenylethyl)-2-[2-(phenylmethoxy)phenyl]-5-[5-(2H-tetrazol-5-yl)-2-thienyl]- (CA INDEX NAME)



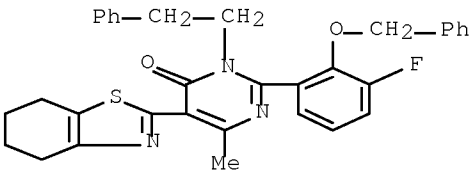
RN 938181-54-5 ZCAPLUS
CN 2-Thiophenecarboxylic acid, 5-[1,6-dihydro-4-methyl-6-oxo-1-(2-phenylethyl)-2-[2-(phenylmethoxy)phenyl]-5-pyrimidinyl]- (CA INDEX NAME)



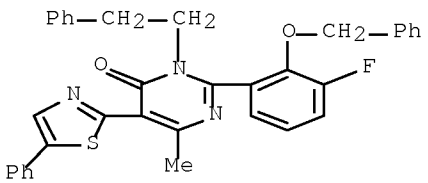
RN 938181-55-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-[5-(hydroxymethyl)-2-thienyl]-6-methyl-3-(2-phenylethyl)-2-[2-(phenylmethoxy)phenyl]- (CA INDEX NAME)



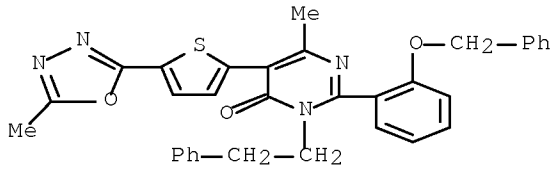
RN 938181-56-7 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-[3-fluoro-2-(phenylmethoxy)phenyl]-6-methyl-3-(2-phenylethyl)-5-(4,5,6,7-tetrahydro-2-benzothiazolyl)- (CA INDEX NAME)



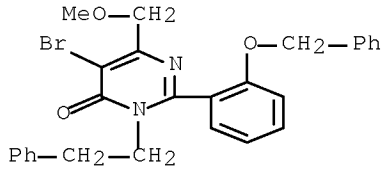
RN 938181-57-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-[3-fluoro-2-(phenylmethoxy)phenyl]-6-methyl-3-(2-phenylethyl)-5-(5-phenyl-2-thiazolyl)- (CA INDEX NAME)



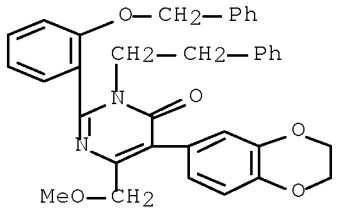
RN 938181-59-0 ZCAPLUS
CN 4(3H)-Pyrimidinone, 6-methyl-5-[5-(5-methyl-1,3,4-oxadiazol-2-yl)-2-thienyl]-3-(2-phenylethyl)-2-[2-(phenylmethoxy)phenyl]- (CA INDEX NAME)



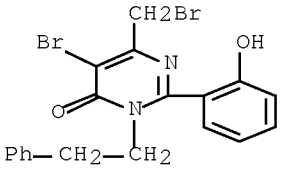
RN 938181-60-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-bromo-6-(methoxymethyl)-3-(2-phenylethyl)-2-[2-(phenylmethoxy)phenyl]- (CA INDEX NAME)



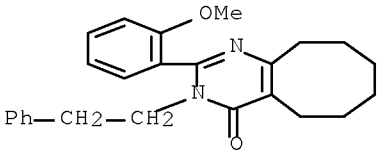
RN 938181-61-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-(2,3-dihydro-1,4-benzodioxin-6-yl)-6-(methoxymethyl)-3-(2-phenylethyl)-2-[2-(phenylmethoxy)phenyl]- (CA INDEX NAME)



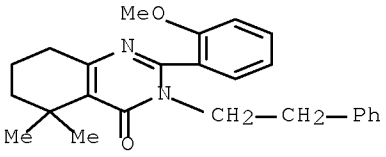
RN 938181-62-5 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-bromo-6-(bromomethyl)-2-(2-hydroxyphenyl)-3-(2-phenylethyl)- (CA INDEX NAME)



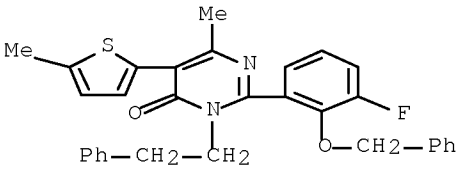
RN 938181-64-7 ZCAPLUS
CN 4(3H)-Cyclooctapyrimidinone, 5,6,7,8,9,10-hexahydro-2-(2-methoxyphenyl)-3-(2-phenylethyl)- (CA INDEX NAME)



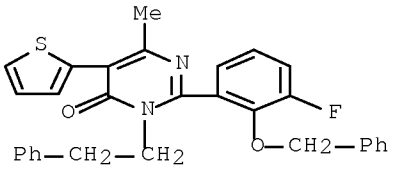
RN 938181-72-7 ZCAPLUS
CN 4(3H)-Quinazolinone, 5,6,7,8-tetrahydro-2-(2-methoxyphenyl)-5,5-dimethyl-3-(2-phenylethyl)- (CA INDEX NAME)



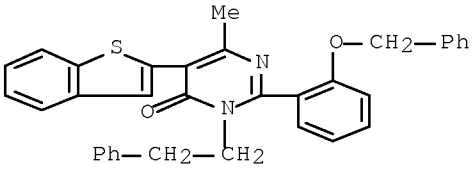
RN 938181-77-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-[3-fluoro-2-(phenylmethoxy)phenyl]-6-methyl-5-(5-methyl-2-thienyl)-3-(2-phenylethyl)- (CA INDEX NAME)



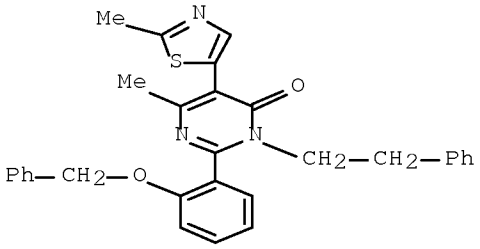
RN 938181-78-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 2-[3-fluoro-2-(phenylmethoxy)phenyl]-6-methyl-3-(2-phenylethyl)-5-(2-thienyl)- (CA INDEX NAME)



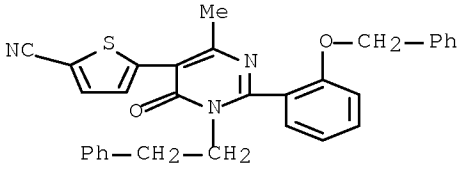
RN 938181-79-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-benzo[b]thien-2-yl-6-methyl-3-(2-phenylethyl)-2-[2-(phenylmethoxy)phenyl]- (CA INDEX NAME)



RN 938181-80-7 ZCAPLUS
CN 4(3H)-Pyrimidinone, 6-methyl-5-(2-methyl-5-thiazolyl)-3-(2-phenylethyl)-2-[2-(phenylmethoxy)phenyl]- (CA INDEX NAME)

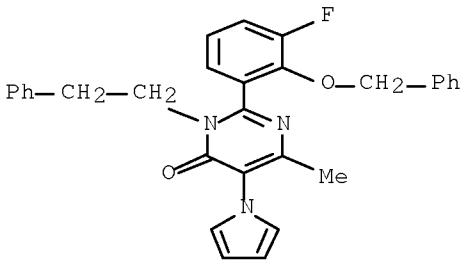


RN 938181-81-8 ZCAPLUS
CN 2-Thiophenecarbonitrile, 5-[1,6-dihydro-4-methyl-6-oxo-1-(2-phenylethyl)-2-[2-(phenylmethoxy)phenyl]-5-pyrimidinyl]- (CA INDEX NAME)



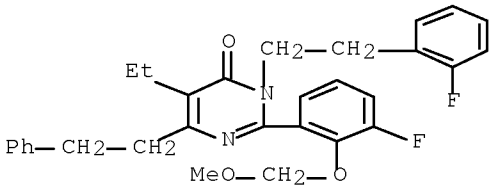
RN 938181-82-9 ZCAPLUS

CN 4(3H)-Pyrimidinone, 2-[3-fluoro-2-(phenylmethoxy)phenyl]-6-methyl-3-(2-phenylethyl)-5-(1H-pyrrol-1-yl)- (CA INDEX NAME)



RN 938181-93-2 ZCAPLUS

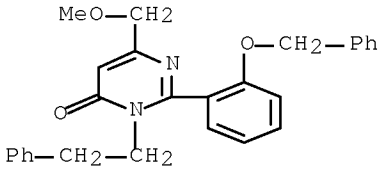
CN 4(3H)-Pyrimidinone, 5-ethyl-2-[3-fluoro-2-(methoxymethoxy)phenyl]-3-[2-(2-fluorophenyl)ethyl]-6-(2-phenylethyl)- (CA INDEX NAME)



IT 938181-84-1 938181-85-2 938181-91-0,
5-Bromo-2-(2-hydroxyphenyl)-6-(methoxymethyl)-3-(2-phenylethyl)-4(3H)-pyrimidinone
RL: RCT (Reactant); RACT (Reactant or reagent)
(starting material; preparation of pyrimidinone derivs. as calcium receptor inhibitors useful in the treatment of bone and mineral diseases)

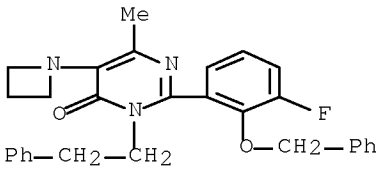
RN 938181-84-1 ZCAPLUS

CN 4(3H)-Pyrimidinone, 6-(methoxymethyl)-3-(2-phenylethyl)-2-[2-(phenylmethoxy)phenyl]- (CA INDEX NAME)

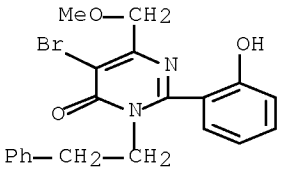


RN 938181-85-2 ZCAPLUS

CN 4(3H)-Pyrimidinone, 5-(1-azetidinyl)-2-[3-fluoro-2-(phenylmethoxy)phenyl]-6-methyl-3-(2-phenylethyl)- (CA INDEX NAME)

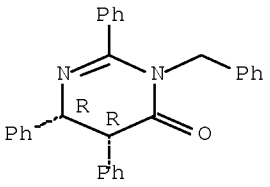


RN 938181-91-0 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-bromo-2-(2-hydroxyphenyl)-6-(methoxymethyl)-3-(2-phenylethyl)- (CA INDEX NAME)



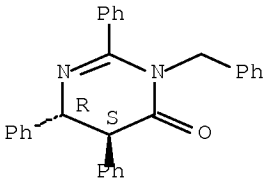
L80 ANSWER 9 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1999:369571 ZCAPLUS Full-text
DOCUMENT NUMBER: 131:116207
TITLE: Substituted 1-benzyl-4-(benzylideneamino)-4-phenylazetidin-2-ones: synthesis and thermal and photochemical reactions
AUTHOR(S): Rossi, Elisabetta; Abbiati, Giorgio; Pini, Elena
CORPORATE SOURCE: Istituto di Chimica Organica, Facolta di Farmacia, Universita degli Studi di Milano, Milan, I-20133, Italy
SOURCE: Tetrahedron (1999), 55(22), 6921-6970
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The title compds. were synthesized from 1,3-diazabuta-1,3-dienes and ketenes. Thermal and photochem. ring expansion reactions to 5,6-dihydro-3H-pyrimidin-4-ones are also described.
IT 198630-84-1P 233257-78-8P 233257-79-9P
233257-80-2P 233257-81-3P 233257-83-5P
233257-86-8P 233257-87-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(1-benzyl-4-(benzylideneamino)-4-phenylazetidin-2-ones and their ring enlargement to dihydropyrimidinones)
RN 198630-84-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5,6-dihydro-2,5,6-triphenyl-3-(phenylmethyl)-, (5R,6R)-rel- (CA INDEX NAME)

Relative stereochemistry.

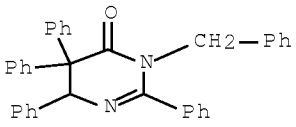


RN 233257-78-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5,6-dihydro-2,5,6-triphenyl-3-(phenylmethyl)-, (5R,6S)-rel- (CA INDEX NAME)

Relative stereochemistry.

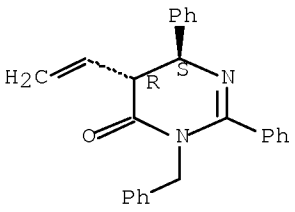


RN 233257-79-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5,6-dihydro-2,5,5,6-tetraphenyl-3-(phenylmethyl)- (CA INDEX NAME)



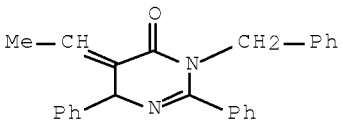
RN 233257-80-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-ethenyl-5,6-dihydro-2,6-diphenyl-3-(phenylmethyl)-, (5R,6S)-rel- (CA INDEX NAME)

Relative stereochemistry.

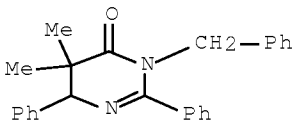


RN 233257-81-3 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-ethylidene-5,6-dihydro-2,6-diphenyl-3-(phenylmethyl)-

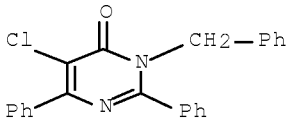
(CA INDEX NAME)



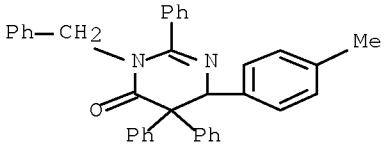
RN 233257-83-5 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5,6-dihydro-5,5-dimethyl-2,6-diphenyl-3-(phenylmethyl)-
(CA INDEX NAME)



RN 233257-86-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5-chloro-2,6-diphenyl-3-(phenylmethyl)- (CA INDEX NAME)



RN 233257-87-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 5,6-dihydro-6-(4-methylphenyl)-2,5,5-triphenyl-3-(phenylmethyl)- (CA INDEX NAME)



REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

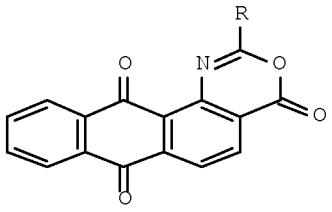
L80 ANSWER 10 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1996:512454 ZCAPLUS Full-text
DOCUMENT NUMBER: 125:221794
ORIGINAL REFERENCE NO.: 125:41453a,41456a
TITLE: Studies on anthraquinone: synthesis and reactions of

2-methyl (phenyl)-4-oxo-1, 3-oxazino[4,5-a]anthraquinone

AUTHOR(S): Kangani, C. O.; Master, H. E.
CORPORATE SOURCE: Nadkarny-Sacasa Research Laboratory, St. Xavier's College, Bombay, 400 001, India

SOURCE: Indian Journal of Heterocyclic Chemistry (1996), 5(4), 261-264
CODEN: IJCHEI; ISSN: 0971-1627
PUBLISHER: Lucknow University, Dep. of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

GI



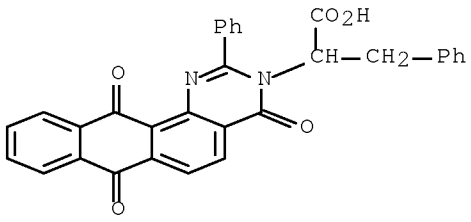
I

AB The reaction of benzoyl chloride and acetic anhydride with 1-amino-9,10-dihydro-9,10-dioxo-2-anthracenecarboxylic acid gave 2-methyl-2H-anthra[1,2-d][1,3]oxazine-4,7,12(1H)-trione I (R = Me) and 2-phenyl-2H-anthra[1,2-d][1,3]oxazine-4,7,12(1H)-trione (R = Ph). Their reaction with hydrazine hydrate, sodium azide, formamide primary amines (aromatic as well as aliphatic), phosphorus pentasulfide and hydroxyl amine hydrochloride have been investigated.

IT 181173-18-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and reactions of anthra[1,2-d][1,3]oxazinetrione)

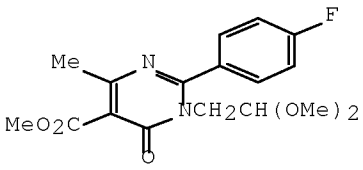
RN 181173-18-2 ZCAPLUS

CN Naphtho[2,3-h]quinazoline-3(4H)-acetic acid, 7,12-dihydro-4,7,12-trioxo-2-phenyl-α-(phenylmethyl)- (CA INDEX NAME)



L80 ANSWER 11 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1993:539183 ZCAPLUS Full-text
DOCUMENT NUMBER: 119:139183
ORIGINAL REFERENCE NO.: 119:24963a,24966a
TITLE: Efficient method for the synthesis of 1,4-disubstituted 5-carbomethoxypyrimidin-6-ones

AUTHOR(S): Veale, Chris A.; Steelman, Gary B.; Chow, Margaret M.
CORPORATE SOURCE: Med. Chem. Dep., ZENECA Inc., Wilmington, DE, 19897, USA
SOURCE: Journal of Organic Chemistry (1993), 58(16), 4490-3
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 119:139183
GI

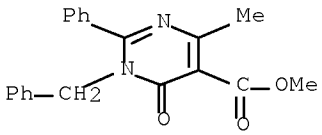


I

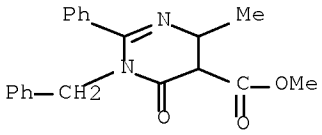
AB A two step procedure is reported for the synthesis of 1,4-disubstituted-5-carbomethoxypyrimidinones. In this procedure an alkylidenemalonate and an N-substituted amidine is condensed to give a 1,4-disubstituted dihydropyrimidinone which is then oxidized using N-bromosuccimide and a radical initiator in the presence of base to give the desired pyrimidinones, e.g. I, in high yields. The method is particularly useful for the preparation of pyrimidinones which contain large substituents at both the 1 and 4-positions of the ring and overcomes the limitations of one of the traditional methods of pyrimidinone synthesis.

IT 149743-06-6P 149743-20-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

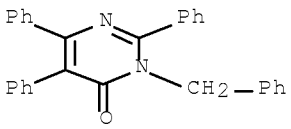
RN 149743-06-6 ZCAPLUS
CN 5-Pyrimidinecarboxylic acid, 1,6-dihydro-4-methyl-6-oxo-2-phenyl-1-(phenylmethyl)-, methyl ester (CA INDEX NAME)



RN 149743-20-4 ZCAPLUS
CN 5-Pyrimidinecarboxylic acid, 1,4,5,6-tetrahydro-4-methyl-6-oxo-2-phenyl-1-(phenylmethyl)-, methyl ester (CA INDEX NAME)

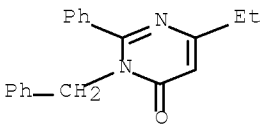


L80 ANSWER 12 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1970:403883 ZCAPLUS Full-text
DOCUMENT NUMBER: 73:3883
ORIGINAL REFERENCE NO.: 73:665a
TITLE: Reactivity of 1,2,4-triphenyl-1-cyano-4-chloro-3-azabuta-1,3-diene. 3-Substituted 2,5,6-triphenyl-4(3H)-pyrimidones. I
AUTHOR(S): Giammanco, Lorenzo; Invidiata, Francesco P.
CORPORATE SOURCE: Ist. Chim. Farm., Univ. Palermo, Palermo, Italy
SOURCE: Annali di Chimica (Rome, Italy) (1970), 60(3), 188-97
CODEN: ANCRAI; ISSN: 0003-4592
DOCUMENT TYPE: Journal
LANGUAGE: Italian
GI For diagram(s), see printed CA Issue.
AB The title azabutadiene is treated with RNH2 (R = alkyl, aryl, PhCH2) to give I. I (R is Ph, 3-methyl-2-pyridyl) are treated with HNO2 to give II. III is treated with primary alkylamines to give II.
IT 26958-76-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 26958-76-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-benzyl-2,5,6-triphenyl- (8CI) (CA INDEX NAME)

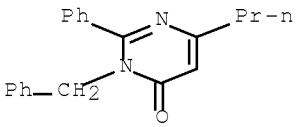


L80 ANSWER 13 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1969:87734 ZCAPLUS Full-text
DOCUMENT NUMBER: 70:87734
ORIGINAL REFERENCE NO.: 70:16397a,16400a
TITLE: Reaction of N-monosubstituted benzamidines with acylacetates and diketene
AUTHOR(S): Sitte, Adolf; Paul, Heinz
CORPORATE SOURCE: Humboldt-Univ. Berlin, Berlin, Fed. Rep. Ger.
SOURCE: Chemische Berichte (1969), 102(2), 615-22
CODEN: CHBEAM; ISSN: 0009-2940
DOCUMENT TYPE: Journal
LANGUAGE: German
OTHER SOURCE(S): CASREACT 70:87734
AB PhC(:NH)NHR (I) were treated with R1OCCH2CO2R2 in alc. solution to give 1-(R-substituted)-4-(R1-substituted)-2-phenyl-6(1H)-pyrimidinones (II) (where R = Me, Pr, PhCH2, or H; and R1 = Me, Et, Pr, iso-Pr, or Ph). Treatment of I (R = PhCH2) with diketene in C6H6 or with excess AcCH2CO2Me in the absence of solvent gave PhC(:NH)N(CH2Ph)COCH2Ac (III), which on treatment with H2O or PhMe gave II (R = PhCH2, R1 = Me). III was hydrolyzed to the starting materials on treatment with alcs.
IT 20959-24-4P 20959-25-5P 20959-26-6P
20959-27-7P 21164-37-4P 22286-10-8P
22286-11-9P 22286-12-0P 22286-13-1P

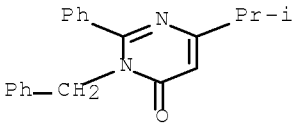
22286-14-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 20959-24-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-benzyl-6-ethyl-2-phenyl- (8CI) (CA INDEX NAME)



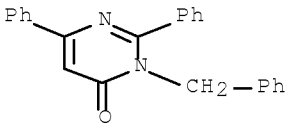
RN 20959-25-5 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-benzyl-2-phenyl-6-propyl- (8CI) (CA INDEX NAME)



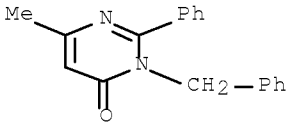
RN 20959-26-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-benzyl-6-isopropyl-2-phenyl- (8CI) (CA INDEX NAME)



RN 20959-27-7 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-benzyl-2,6-diphenyl- (8CI) (CA INDEX NAME)



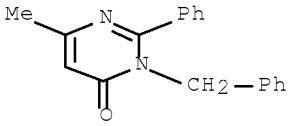
RN 21164-37-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-benzyl-6-methyl-2-phenyl- (8CI) (CA INDEX NAME)



RN 22286-10-8 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-benzyl-6-methyl-2-phenyl-, monopicrate (8CI) (CA INDEX NAME)

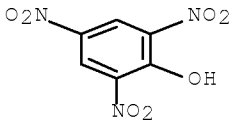
CM 1

CRN 21164-37-4
CMF C18 H16 N2 O



CM 2

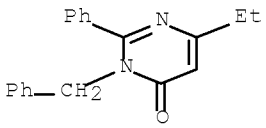
CRN 88-89-1
CMF C6 H3 N3 O7



RN 22286-11-9 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-benzyl-6-ethyl-2-phenyl-, monopicrate (8CI) (CA INDEX NAME)

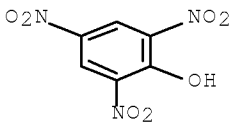
CM 1

CRN 20959-24-4
CMF C19 H18 N2 O



CM 2

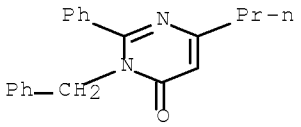
CRN 88-89-1
CMF C6 H3 N3 O7



RN 22286-12-0 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-benzyl-2-phenyl-6-propyl-, monopicrate (8CI) (CA INDEX NAME)

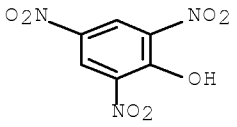
CM 1

CRN 20959-25-5
CMF C20 H20 N2 O



CM 2

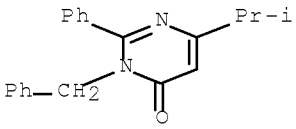
CRN 88-89-1
CMF C6 H3 N3 O7



RN 22286-13-1 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-benzyl-6-isopropyl-2-phenyl-, monopicrate (8CI) (CA INDEX NAME)

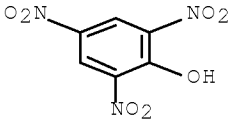
CM 1

CRN 20959-26-6
CMF C20 H20 N2 O



CM 2

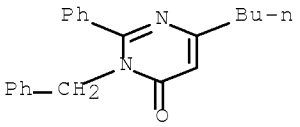
CRN 88-89-1
CMF C6 H3 N3 O7



RN 22286-14-2 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-benzyl-6-butyl-2-phenyl-, monopicrate (8CI) (CA INDEX NAME)

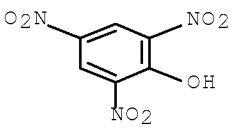
CM 1

CRN 47349-86-0
CMF C21 H22 N2 O



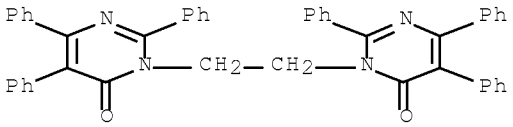
CM 2

CRN 88-89-1
CMF C6 H3 N3 O7



L80 ANSWER 14 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1969:449884 ZCAPLUS Full-text

DOCUMENT NUMBER: 71:49884
ORIGINAL REFERENCE NO.: 71:9172h,9173a
TITLE: Conversion of oxazinones to pyrimidines
AUTHOR(S): Giammanco, Lorenzo
CORPORATE SOURCE: Univ. Palermo, Palermo, Italy
SOURCE: Atti della Accademia di Scienze, Lettere e Arti di Palermo, Parte 1: Scienze (1968), Volume Date 1966-1967, 27, 469-83
CODEN: AASLAN; ISSN: 0365-0448
DOCUMENT TYPE: Journal
LANGUAGE: Italian
GI For diagram(s), see printed CA Issue.
AB I are prepared from 2,4,5-triphenyl-1,3-oxazin-6-one (II); 3,3'-ethylenebis(2,5,6-triphenylpyrimidin-4-one) (III) and 3-amino compds. IV are also prepared A mixture of 0.01 mole II, 0.05 mole appropriate amine RNH2, and 150 ml. alc. is agitated to give 3-methyl-2,5,6- triphenylpyrimidin-4-one, m. 230°, and the following I (R and m.p. given): Et, 172°; CH2CH2NEt2, 146°; CH2CH2NH2, 186°; CH2CH2OH, 235-7°. A mixture of 0.92 g. H2NCH2CH2NH2, 0.81 g. II, and 150 ml. alc. is refluxed 15-20 hrs. to give III, m. 342°. A mixture of 1 g. II and 2 ml. Ph-NHNH2 is heated 3-4 hrs. to give I (R = H), m. 298°. II (3 g.) is treated with 25 ml. 85% N2H4.H2O in 500 ml. alc. 25-6 hrs. to give 2,5,6-triphenyl-4-aminopyrimidin-4-one (V), m. 190°, which is converted to IV (R = R1 = Ac) (VI), m. 185°. VI (1 g.) is refluxed with 15 ml. POCl3 to give IV (R = H, R1 = Ac) (VII), m. 258-60°; VII (m. 260°) is also prepared from VI and KOH. V (3.25 g.) is acylated (1.6 g. BzCl) to give IV (R = H, R1 = Bz), m. 245-7°, which is converted to IV (R = Ac, R1 = Bz), m. 190°. V (2 g.) is heated with 2 g. BzH and 20 ml. HCl-saturated alc. to give 3-(benzylideneamino)-2,5,6-triphenylpyrimidin-4-one, m. 175°. A mixture of V and NaNO2 is heated to give 2,5,6-triphenyl-4- hydroxyphyrimidine, m. 306°.
IT 23413-51-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 23413-51-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3,3'-ethylenebis[2,5,6-triphenyl- (8CI) (CA INDEX NAME)

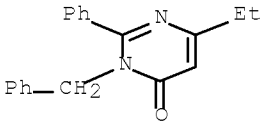


L80 ANSWER 15 OF 22 ZCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1969:11666 ZCAPLUS Full-text
DOCUMENT NUMBER: 70:11666
ORIGINAL REFERENCE NO.: 70:2187a,2190a
TITLE: Heterocycles. III. Reaction of monosubstituted benzamidines with acylacetic acid esters
AUTHOR(S): Paul, Heinz; Sitte, Adolf
CORPORATE SOURCE: Humboldt-Univ. Berlin, Berlin, Fed. Rep. Ger.
SOURCE: Zeitschrift fuer Chemie (1968), 8(9), 336-7
CODEN: ZECEAL; ISSN: 0044-2402
DOCUMENT TYPE: Journal
LANGUAGE: German
GI For diagram(s), see printed CA Issue.

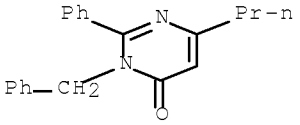
AB PhC(:NH)NHR were treated with R1COCH2CO2R2 in R2OH to give substituted 2-phenyl-1,6-dihydropyrimidin-6-ones (I) (where R = Me, Pr, or PhCH2; and R1 = Me, Et, Pr, iso-Pr, or Ph). In the absence of solvent, PhC-(:NH)N(CH2Ph)COCH2Ac was obtained, which was converted to I (R = PhCH2, R1 = Me) on heating.

IT 20959-24-4P 20959-25-5P 20959-26-6P
20959-27-7P 21164-37-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

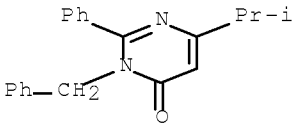
RN 20959-24-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-benzyl-6-ethyl-2-phenyl- (8CI) (CA INDEX NAME)



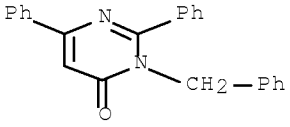
RN 20959-25-5 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-benzyl-2-phenyl-6-propyl- (8CI) (CA INDEX NAME)



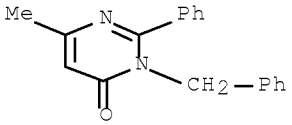
RN 20959-26-6 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-benzyl-6-isopropyl-2-phenyl- (8CI) (CA INDEX NAME)



RN 20959-27-7 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-benzyl-2,6-diphenyl- (8CI) (CA INDEX NAME)



RN 21164-37-4 ZCAPLUS
CN 4(3H)-Pyrimidinone, 3-benzyl-6-methyl-2-phenyl- (8CI) (CA INDEX NAME)



L80 ANSWER 16 OF 22 PROUSDDR COPYRIGHT 2008 PROUS SCIENCE on STN
ACCESSION NUMBER: 2005:7248 PROUSDDR Full-text
DOCUMENT NUMBER: 399143
CHEMICAL NAME: 5-Ethyl-3-(2-(2-fluorophenyl)ethyl)-2-(2-hydroxyphenyl)-6-methylpyrimidin-4(3H)-one
CAS REGISTRY NUMBER: 780771-44-0
MOLECULAR FORMULA: C21 H21 F N2 O2
HIGHEST DEV. PHASE: PRECLINICAL
ORIGINATOR: GlaxoSmithKline
NPS Pharmaceuticals
CLASSIFICATION CODE: Bone Formation Stimulants
OTHER SOURCE: SYNTHLINE 2006000519
ENTRY DATE: Entered STN: 3 Oct 2005
Last Updated on STN: 1 Apr 2008

STRUCTURE:

/ BINARY DATA / jaisle363res001.TIF

PROUS REFERENCES:
RefID: 909690 (Text Available)
Drug Data Report, Vol. 27, No. 6, pp 585, 2005

REFERENCE TEXT: RefID: 909690
ACTION - Calcium receptor antagonist, a calcilytic compound (IC50 = 0.097 mcM) proven to induce a rapid but transient dose-related increase in plasma parathyroid hormone levels when given to rats (1 or 3 mcM/kg i.v.). Potentially useful for the treatment of osteoporosis.

PATENT REFERENCES:

TITLE: Pyrimidinone compounds as calcilytics
INVENTOR(S): Wang, W.; Balandrin, M.F.; Yamashita, D.S.; Fox, J.; Huang, G.; Shcherbakova, I.V.; Geoffroy, O.; Marquis, R.; Luengo, J.
PATENT ASSIGNEE(S): GlaxoSmithKline
PATENT ASSIGNEE(S): NPS Pharmaceuticals
PATENT INFORMATION: EP 1615897 20060118
JP 2006522159 20060928
JP 2006522160 20060928
US 2007197555 20070823
WO 2004092120 20041028
WO 2004092121 20041028

PRIORITY INFORMATION: US 2003-460859 20030407
US 2003-479323 20030618
US 2006-552363 20061120

REFERENCES:
(1) RefID: 905707, Periodic Publication
"Design, new synthesis, and calcilytic activity of substituted 3H-pyrimidin-4-ones"
Shcherbakova, I.; Huang, G.; Geoffroy, O.J.; et al., Bioorg Med Chem Lett, Vol. 15, No. 10, pp 2537, 2005

START LOCAL KERMIT RECEIVE PROCESS

BINARY DATA HAS BEEN DOWNLOADED TO MULTIPLE FILES 'IMAGEnnn.TIF'

L80 ANSWER 17 OF 22 SYNTHLINE COPYRIGHT 2008 PROUS SCIENCE on STN
ACCESSION NUMBER: 2006:519 SYNTHLINE
ENTRY NUMBER: 399143
CHEMICAL NAME: 5-Ethyl-3-(2-(2-fluorophenyl)ethyl)-2-(2-hydroxyphenyl)-6-methylpyrimidin-4(3H)-one
CAS REGISTRY NO.: 780771-44-0
MOLECULAR FORMULA: C21 H21 F N2 O2
MOLECULAR WEIGHT: 352.41
CLASSIFICATION CODE: Bone Diseases, Treatment of; Bone Formation Stimulants; METABOLIC DRUGS; Treatment of Osteoporosis; Calcium-Sensing Receptor (CaSR) Antagonists; Parathyroid Hormone Secretion Stimulants
HIGHEST DEV. PHASE: Preclinical
COMPANY: GlaxoSmithKline; NPS Pharmaceuticals
ENTRY DATE: Entered STN: 15 Jun 2006
Last Updated on STN: 16 Jun 2008

STRUCTURE:

/ BINARY DATA / jaisle363res002.TIF

REACTION: 39914301a
TEXT:
Ketalization of ethyl 2-ethyl-3-oxobutyrate (I) with ethylene glycol and p-TsOH, followed by basic hydrolysis of the resultant ketal ester (II) leads to the carboxylic acid (III). After activation of (III) as the corresponding acid chloride (IV), coupling with 2-fluorophenethylamine (V) provides the ketal amide (VI). The ethylene ketal (VI) is then hydrolyzed under acidic conditions to furnish the keto amide (VII), which is then converted to enamine (VIII) by reaction with ammonia in the presence of AlCl3. Acylation of enamine (VIII) with acetyl salicyl chloride (IX) produces the enediamide (X), which is finally hydrolyzed and cyclized to the target pyrimidinone upon treatment with KOH in aqueous EtOH (1,2).

/ BINARY DATA / jaisle363res003.TIF
TITLE: Design, new synthesis, and calcilytic activity of substituted 3H-pyrimidin-4-ones
AUTHOR(S): Shcherbakova, I.; Huang, G.; Geoffroy, O.J.; et al
SOURCE: Bioorg Med Chem Lett (2005), 15(10), 2537

TITLE: Pyrimidinone compounds as calcilytics
INVENTOR(S): Luengo, J.; Marquis, R.; Geoffroy, O.; Shcherbakova, I.V.; Huang, G.; Fox, J.; Yamashita, D.S.; Balandrin,

M.F.; Wang, W.
PATENT ASSIGNEE(S): GlaxoSmithKline Inc.; NPS Pharmaceuticals, Inc.
PATENT INFORMATION: EP 1615897; WO 2004092120; WO 2004092121

REACTANT IDENTIFIER: (IX) 16900
CHEMICAL NAME: Acetylsalicyloyl chloride; 2-(chlorocarbonyl)phenyl acetate
CAS REGISTRY NO.: 5538-51-2
MOLECULAR FORMULA: C9 H7 Cl O3
MOLECULAR WEIGHT: 198.61
COMPANY: Aldrich; Alfa Aesar; Fluka; Lancaster Synthesis Inc.; Morre-Tec Industries, Inc.; Zhejiang Genglou Chemical Industry Co., Ltd.

REACTANT IDENTIFIER: (V) 31333
CHEMICAL NAME: 2-(2-fluorophenyl)-1-ethanamine; 2-fluorophenethylamine
MOLECULAR FORMULA: C8 H10 F N
MOLECULAR WEIGHT: 139.17
COMPANY: Aldrich; Donboo Amino Acid Company Ltd.

REACTANT IDENTIFIER: (I) 67774
CHEMICAL NAME: ethyl 2-ethyl-3-oxobutanoate
CAS REGISTRY NO.: 607-97-6
MOLECULAR FORMULA: C8 H14 O3
MOLECULAR WEIGHT: 158.2
COMPANY: Acros Organics; Aldrich; Fine & Performance Chemicals Ltd.; Fluka; Lancaster Synthesis Inc.; Minakem; MP Biomedicals; Pfaltz & Bauer, Inc.; Syntai Chemicals & Pharmaceuticals, Ltd.; Whyte Chemicals Limited

REACTANT IDENTIFIER: (II) 901142
CHEMICAL NAME: ethyl 2-(2-methyl-1,3-dioxolan-2-yl)butanoate
MOLECULAR FORMULA: C10 H18 O4
MOLECULAR WEIGHT: 202.25

REACTANT IDENTIFIER: (III) 901143
CHEMICAL NAME: 2-(2-methyl-1,3-dioxolan-2-yl)butanoic acid
MOLECULAR FORMULA: C8 H14 O4
MOLECULAR WEIGHT: 174.2

REACTANT IDENTIFIER: (IV) 901144
CHEMICAL NAME: 2-(2-methyl-1,3-dioxolan-2-yl)butanoyl chloride
MOLECULAR FORMULA: C8 H13 Cl O3
MOLECULAR WEIGHT: 192.64

REACTANT IDENTIFIER: (VI) 901145
CHEMICAL NAME: N-(2-fluorophenethyl)-2-(2-methyl-1,3-dioxolan-2-yl)butanamide
MOLECULAR FORMULA: C16 H22 F N O3
MOLECULAR WEIGHT: 295.36

REACTANT IDENTIFIER: (VII) 901146
CHEMICAL NAME: 2-ethyl-N-(2-fluorophenethyl)-3-oxobutanamide
MOLECULAR FORMULA: C14 H18 F N O2
MOLECULAR WEIGHT: 251.3

REACTANT IDENTIFIER: (VIII) 901147
CHEMICAL NAME: (Z)-3-amino-2-ethyl-N-(2-fluorophenethyl)-2-butenamide
MOLECULAR FORMULA: C14 H19 F N2 O
MOLECULAR WEIGHT: 250.32

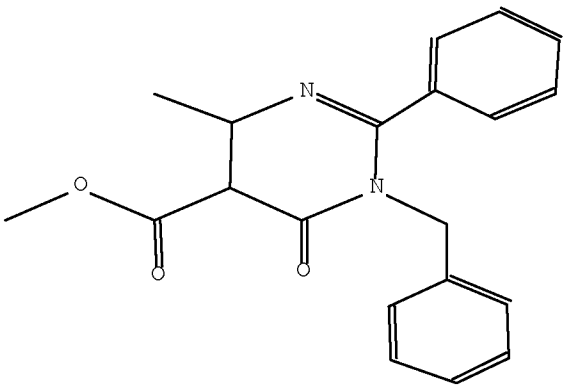
REACTANT IDENTIFIER: (X) 901148
CHEMICAL NAME: 2-((((Z)-2-(((2-fluorophenethyl)amino)carbonyl)-1-methyl-1-butenyl)amino)carbonyl)phenyl acetate
MOLECULAR FORMULA: C23 H25 F N2 O4
MOLECULAR WEIGHT: 412.47

START LOCAL KERMIT RECEIVE PROCESS

BINARY DATA HAS BEEN DOWNLOADED TO MULTIPLE FILES 'IMAGEnnn.TIF'

L80 ANSWER 18 OF 22 BEILSTEIN COPYRIGHT 2008 BEILSTEIN MDL on STN

Beilstein Records (BRN):	6347051
Chemical Name (CN):	1-benzyl-4-methyl-6-oxo-2-phenyl-1,4,5,6-tetrahydro-pyrimidine-5-carboxylic acid methyl ester
Autonom Name (AUN):	1-benzyl-4-methyl-6-oxo-2-phenyl-1,4,5,6-tetrahydro-pyrimidine-5-carboxylic acid methyl ester
Molec. Formula (MF):	C20 H20 N2 O3
Molecular Weight (MW):	336.39
Lawson Number (LN):	29410, 14140, 289
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	5512175
Tautomer ID (TAUTID):	6021196
Beilstein Citation (BSO):	6-25
Entry Date (DED):	1994/01/24
Update Date (DUPD):	1994/10/31



Field Availability:

Code	Name	Occurrence

BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

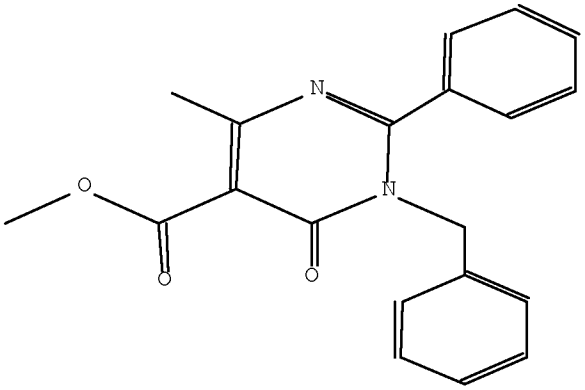
Code	Name	Occurrence
RX	Reaction Documents	2
RXREA	Substance is Reaction Reactant	1
RXPRO	Substance is Reaction Product	1

All References:
ALLREF

1. Veale, Chris A.; Steelman, Gary B.; Chow, Margaret M., J.Org.Chem., CODEN: JOCEAH, 58(16), <1993>, 4490-4493; BABS-5817151

L80 ANSWER 19 OF 22 BEILSTEIN COPYRIGHT 2008 BEILSTEIN MDL on STN

Beilstein Records (BRN):	6345886
Chemical Name (CN):	1-benzyl-4-methyl-6-oxo-2-phenyl-1,6-dihydro-pyrimidine-5-carboxylic acid methyl ester
Autonom Name (AUN):	1-benzyl-4-methyl-6-oxo-2-phenyl-1,6-dihydro-pyrimidine-5-carboxylic acid methyl ester
Molec. Formula (MF):	C20 H18 N2 O3
Molecular Weight (MW):	334.37
Lawson Number (LN):	29410, 14140, 289
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	5516615
Tautomer ID (TAUTID):	6025119
Beilstein Citation (BSO):	6-25
Entry Date (DED):	1994/01/24
Update Date (DUPD):	1994/10/31



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	3
FS	File Segment	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

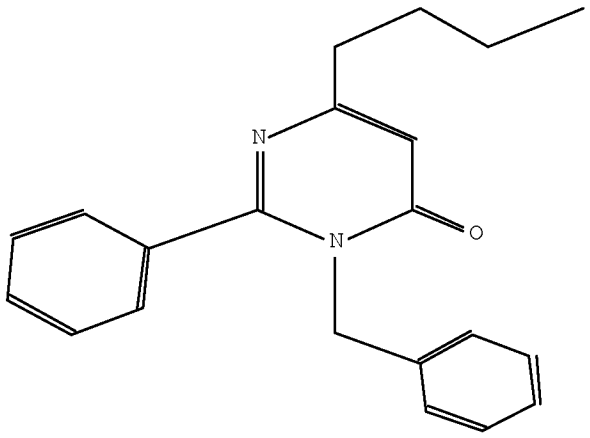
All References:
ALLREF

1. Veale, Chris A.; Steelman, Gary B.; Chow, Margaret M., J.Org.Chem., CODEN: JOCEAH, 58(16), <1993>, 4490-4493; BABS-5817151

L80 ANSWER 20 OF 22 BEILSTEIN COPYRIGHT 2008 BEILSTEIN MDL on STN

Beilstein Records (BRN):	1594504
Beilstein Pref. RN (BPR):	47349-86-0
CAS Reg. No. (RN):	47349-86-0
Chemical Name (CN):	3-benzyl-6-butyl-2-phenyl-3H-pyrimidin-4-one
Autonom Name (AUN):	3-benzyl-6-butyl-2-phenyl-3H-pyrimidin-4-one

Molec. Formula (MF):	C21 H22 N2 O
Molecular Weight (MW):	318.42
Lawson Number (LN):	28722, 14140
Compound Type (CTYPE):	heterocyclic
Constitution ID (CONSID):	1444308
Tautomer ID (TAUTID):	1493639
Beilstein Citation (BSO):	5-24-03-00553
Entry Date (DED):	1988/11/30
Update Date (DUPD):	1992/09/09



Field Availability:

Code	Name	Occurrence
BRN	Beilstein Records	1
BPR	Beilstein Preferred RN	1
RN	CAS Registry Number	1
CN	Chemical Name	1
AUN	Autonomname	1
MF	Molecular Formula	1
FW	Formular Weight	1
LN	Lawson Number	2
CTYPE	Compound Type	1
CONSID	Constitution ID	1
TAUTID	Tautomer ID	1
BSO	Beilstein Citation	1
ED	Entry Date	1
UPD	Update Date	1

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1
RXPRO	Substance is Reaction Product	1

All References:
ALLREF

1. Sitte,A.; Paul,H., Chem.Ber., CODEN: CHBEAM, 102(2), <1969>, 615-622

L80 ANSWER 21 OF 22 BABS COPYRIGHT 2008 BEILSTEIN MDL on STN
ACCESSION NUMBER: 6184091 BABS Full-text
TITLE: Substituted 1-Benzyl-4-(benzylideneimino)-4-phenylazetidin-2-ones: Synthesis, Thermal and Photochemical Reactions
AUTHOR(S): Rossi, Elisabetta; Abbiati, Giorgio; Pini, Elena
SOURCE: Tetrahedron (1999), 55(22), 6961 - 6970
CODEN: TETRAB
DOCUMENT TYPE: Journal
LANGUAGE: English
SUMMARY LANGUAGE: English
ABSTRACT: The title compounds were synthesized from 1,3-diazabuta-1,3-dienes and ketenes. Thermal and photochemical ring expansion reactions to 5,6-dihydro-3H-pyrimidin-4-ones are also described.

L80 ANSWER 22 OF 22 BABS COPYRIGHT 2008 BEILSTEIN MDL on STN
ACCESSION NUMBER: 5924807 BABS Full-text
TITLE: Synthesis of N-Substituted Oxo- and Thioxopyrimidines from 1,2,4-Dithiazolium Salts
AUTHOR(S): Holzer, Max; Dobner, Bodo; Briel, Detlef
SOURCE: Liebigs Ann.Chem. (1994), (9), 895-900
CODEN: LACHDL
DOCUMENT TYPE: Journal
LANGUAGE: German
SUMMARY LANGUAGE: English
ABSTRACT: 2,4-Diaryl-substituted 1,3-thiazine-5-carbonitriles 5, 6, obtained by reaction of 1,2,4-dithiazolium salts 1 with activated cyanoacetates, undergo ring transformations in the presence of primary and secondary amines.Thus, 5 and 6 react with primary amines under mild conditions to give hardly accessible N-3-substituted oxopyrimidine- or thioxopyrimidine-5-carbonitriles 11, 16, with secondary amines to give N-3-unsubstituted pyrimidine derivatives 14, 19 and with diamines to give imidazo<1,2-c>pyrimidines or pyrimido<1,2-c>pyrimidines 23a, b.After alkylation of

1,3-thiazines 6, highly reactive 1,3-thiazinium salts 8 can be isolated. CONTROLLED TERM(S): 1,3-Thiazines / Pyrimidines / Thiazinium salts

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=>  d his full

     (FILE 'HOME' ENTERED AT 11:32:18 ON 04 AUG 2008)

     FILE 'REGISTRY' ENTERED AT 11:32:23 ON 04 AUG 2008
L1              STRUCTURE UPLOADED
L2            5 SEA SSS SAM L1
                D SCA
                D STAT QUE L2
L3         3630 SEA SSS FUL L1
                SAVE TEMP L3 JAI363STR1L/A
L4              STRUCTURE UPLOADED
L5           45 SEA SUB=L3 SSS SAM L4
                D SCA
L6              STRUCTURE UPLOADED
L7           33 SEA SUB=L3 SSS SAM L6
L8          644 SEA SUB=L3 SSS FUL L6
                SAVE TEMP JAI363STR6L/A L8

     FILE 'ZCAPLUS' ENTERED AT 11:51:14 ON 04 AUG 2008
L9           15 SEA ABB=ON  PLU=ON  L8
                D SCA

     FILE 'REGISTRY' ENTERED AT 11:51:47 ON 04 AUG 2008
L10             ANALYZE PLU=ON  L8 1- LC :       9 TERMS
                D

     FILE 'CASREACT' ENTERED AT 11:54:04 ON 04 AUG 2008
L11           5 SEA ABB=ON  PLU=ON  L8

     FILE 'TOXCENTER' ENTERED AT 11:54:38 ON 04 AUG 2008

     FILE 'REGISTRY' ENTERED AT 11:55:35 ON 04 AUG 2008
L12          26 SEA ABB=ON  PLU=ON  L8 AND TOXCENTER/LC

     FILE 'TOXCENTER' ENTERED AT 11:55:54 ON 04 AUG 2008
L13           1 SEA ABB=ON  PLU=ON  L12
                D L10

     FILE 'REGISTRY' ENTERED AT 11:56:36 ON 04 AUG 2008
L14           1 SEA ABB=ON  PLU=ON  L8 AND BEILSTEIN/LC NOT CAPLUS/LC
                D SCA
L15           1 SEA ABB=ON  PLU=ON  L8 AND P?/LC
L16           1 SEA ABB=ON  PLU=ON  L8 AND SY?/LC

     FILE 'PROUSDDR' ENTERED AT 11:58:15 ON 04 AUG 2008
L17           1 SEA ABB=ON  PLU=ON  L15

     FILE 'SYNTHLINE' ENTERED AT 11:58:30 ON 04 AUG 2008
L18           1 SEA ABB=ON  PLU=ON  L16
                D ALL

     FILE 'PROUSDDR' ENTERED AT 11:59:09 ON 04 AUG 2008
                D ALL L17

     FILE 'SYNTHLINE' ENTERED AT 11:59:12 ON 04 AUG 2008

     FILE 'BEILSTEIN' ENTERED AT 11:59:32 ON 04 AUG 2008
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L19           0 SEA SSS SAM L6
L20           1 SEA SSS SAM L1
L21           1 SEA SSS SAM L1 AND L6
L22          39 SEA SSS FUL L1 AND L6
L23          29 SEA ABB=ON  PLU=ON  L22 AND BABSAN/FA
                SEL BABSAN

     FILE 'BABS' ENTERED AT 12:02:36 ON 04 AUG 2008
L24           5 SEA ABB=ON  PLU=ON  (6499421/BABSAN OR 6184091/BABSAN OR
                5924807/BABSAN OR 6073136/BABSAN OR 6308281/BABSAN)

     FILE 'BEILSTEIN' ENTERED AT 12:02:50 ON 04 AUG 2008
L25           1 SEA ABB=ON  PLU=ON  L14
L26          10 SEA ABB=ON  PLU=ON  L22 NOT L23
L27           8 SEA ABB=ON  PLU=ON  L26 AND RN/FA
L28           2 SEA ABB=ON  PLU=ON  L26 NOT L27
L29           3 SEA ABB=ON  PLU=ON  L25 OR L28

     FILE 'ZCAPLUS, BABS' ENTERED AT 12:04:10 ON 04 AUG 2008
L30          17 DUP REM L9 L24 (3 DUPLICATES REMOVED)
                    ANSWERS '1-15' FROM FILE ZCAPLUS
                    ANSWERS '16-17' FROM FILE BABS

     FILE 'REGISTRY' ENTERED AT 12:04:33 ON 04 AUG 2008
L31         199 SEA ABB=ON  PLU=ON  L8 AND CHEMCATS/LC NOT CAPLUS/LC

     FILE 'CHEMCATS' ENTERED AT 12:05:05 ON 04 AUG 2008
L32         403 SEA ABB=ON  PLU=ON  L31
L33           0 SEA ABB=ON  PLU=ON  L32 AND PY/FA

     FILE 'STNGUIDE' ENTERED AT 12:05:43 ON 04 AUG 2008

     FILE 'CHEMCATS' ENTERED AT 12:08:18 ON 04 AUG 2008
L34           0 SEA ABB=ON  PLU=ON  L32 AND PD<2003
L35         403 SEA ABB=ON  PLU=ON  L32 AND PD>2003
L36           0 SEA ABB=ON  PLU=ON  L32 AND ED<2003
L37         403 SEA ABB=ON  PLU=ON  L32 AND ED>2003
L38           0 SEA ABB=ON  PLU=ON  L32 AND ED<2004
L39           0 SEA ABB=ON  PLU=ON  L32 AND PD<2004
L40           0 SEA ABB=ON  PLU=ON  L32 AND PD<2005
L41           0 SEA ABB=ON  PLU=ON  L32 AND ED<2005

     FILE 'ZCAPLUS' ENTERED AT 12:11:21 ON 04 AUG 2008
L42         183 SEA ABB=ON  PLU=ON  SHCHERBAKOVA I?/AU
L43          71 SEA ABB=ON  PLU=ON  BALANDRIN M?/AU
L44        5459 SEA ABB=ON  PLU=ON  HUANG G?/AU
L45          30 SEA ABB=ON  PLU=ON  GEOFFROY O?/AU
L46        3199 SEA ABB=ON  PLU=ON  FOX J?/AU
L47         307 SEA ABB=ON  PLU=ON  MARQUIS R?/AU
L48         194 SEA ABB=ON  PLU=ON  YAMASHITA D?/AU
L49         182 SEA ABB=ON  PLU=ON  LUENGO J?/AU
L50       29811 SEA ABB=ON  PLU=ON  WANG W?/AU
L51           7 SEA ABB=ON  PLU=ON  L42 AND (L43 OR L44 OR L45 OR L46 OR L47
                OR L48 OR L49 OR L50)
L52           7 SEA ABB=ON  PLU=ON  L43 AND (L44 OR L45 OR L46 OR L47 OR L48
                OR L49 OR L50)
L53         270 SEA ABB=ON  PLU=ON  L44 AND (L45 OR L46 OR L47 OR L48 OR L49
                OR L50)
L54           3 SEA ABB=ON  PLU=ON  L45 AND (L46 OR L47 OR L48 OR L49 OR L50)
L55           2 SEA ABB=ON  PLU=ON  L46 AND (L47 OR L48 OR L49 OR L50)
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L56          25 SEA ABB=ON  PLU=ON  L47 AND (L48 OR L49 OR L50)
L57          10 SEA ABB=ON  PLU=ON  L48 AND (L49 OR L50)
L58           1 SEA ABB=ON  PLU=ON  L49 AND L50
L59          40 SEA ABB=ON  PLU=ON  (L51 OR L52 OR L54 OR L55 OR L56 OR L57 OR
                L58)
L60           5 SEA ABB=ON  PLU=ON  L51 AND (L52 OR L53 OR L54 OR L55 OR L56
                OR L57 OR L58)
L61           3 SEA ABB=ON  PLU=ON  L52 AND (L53 OR L54 OR L55 OR L56 OR L57
                OR L58)
L62           3 SEA ABB=ON  PLU=ON  L53 AND (L54 OR L55 OR L56 OR L57 OR L58)
L63           1 SEA ABB=ON  PLU=ON  L54 AND (L55 OR L56 OR L57 OR L58)
L64           2 SEA ABB=ON  PLU=ON  L55 AND (L56 OR L57 OR L58)
L65           3 SEA ABB=ON  PLU=ON  L56 AND (L57 OR L58)
L66           1 SEA ABB=ON  PLU=ON  L57 AND L58
L67           8 SEA ABB=ON  PLU=ON  (L60 OR L61 OR L62 OR L63 OR L64 OR L65 OR
                L66)
L68        7528 SEA ABB=ON  PLU=ON  ?PYRIMIDINON?/BI
L69          40 SEA ABB=ON  PLU=ON  (L42 OR L43 OR L44 OR L45 OR L46 OR L47 OR
                L48 OR L49 OR L50) AND L68
L70          43 SEA ABB=ON  PLU=ON  L67 OR L69
L71          77 SEA ABB=ON  PLU=ON  ?CALCILYT?/BI
L72           6 SEA ABB=ON  PLU=ON  L69 AND L71

     FILE 'REGISTRY' ENTERED AT 12:17:50 ON 04 AUG 2008

     FILE 'ZCAPLUS' ENTERED AT 12:17:55 ON 04 AUG 2008
                D STAT QUE L67
                D STAT QUE L69
                D STAT QUE L72
L73          43 SEA ABB=ON  PLU=ON  L67 OR L69 OR L72

     FILE 'MEDLINE, EMBASE, BIOSIS' ENTERED AT 12:18:28 ON 04 AUG 2008
L74           7 SEA ABB=ON  PLU=ON  L67

     FILE 'WPIX' ENTERED AT 12:19:13 ON 04 AUG 2008
L75           6 SEA ABB=ON  PLU=ON  (L60 OR L61 OR L62 OR L63 OR L64 OR L65 OR
                L66)

     FILE 'REGISTRY' ENTERED AT 12:20:02 ON 04 AUG 2008
                D STAT QUE L67
                D STAT QUE L69
                D STAT QUE L72

     FILE 'REGISTRY' ENTERED AT 12:20:36 ON 04 AUG 2008

     FILE 'ZCAPLUS' ENTERED AT 12:20:42 ON 04 AUG 2008
                E US2007-728393/APPS
L76           1 SEA ABB=ON  PLU=ON  US2007-728393/AP
                D SCA
                SEL RN

     FILE 'REGISTRY' ENTERED AT 12:24:17 ON 04 AUG 2008
L77          32 SEA ABB=ON  PLU=ON  (131223-60-4/BI OR 135-77-3/BI OR 2150-47-2
                /BI OR 26510-91-8/BI OR 326606-12-6/BI OR 326606-24-0/BI OR
                5556-86-5/BI OR 67828-44-8/BI OR 67828-69-7/BI OR 811788-09-7/B
                I OR 811788-11-1/BI OR 811788-14-4/BI OR 811788-16-6/BI OR
                811788-17-7/BI OR 811788-18-8/BI OR 811788-19-9/BI OR 811788-20
                -2/BI OR 811788-21-3/BI OR 867-13-0/BI OR 884646-68-8/BI OR
                884646-69-9/BI OR 884646-70-2/BI OR 884646-71-3/BI OR 884646-72
                -4/BI OR 884646-73-5/BI OR 884646-74-6/BI OR 884646-75-7/BI OR
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                884646-76-8/BI OR 884646-77-9/BI OR 884646-78-0/BI OR 884646-90
                -6/BI OR 936478-90-9/BI)
                D SCA

     FILE 'STNGUIDE' ENTERED AT 12:30:24 ON 04 AUG 2008

     FILE 'REGISTRY' ENTERED AT 12:37:40 ON 04 AUG 2008

     FILE 'ZCAPLUS' ENTERED AT 12:37:44 ON 04 AUG 2008
                D STAT QUE L67
                D STAT QUE L69
                D STAT QUE L72
L78           43 SEA ABB=ON  PLU=ON  L67 OR L69 OR L72

     FILE 'MEDLINE, EMBASE, BIOSIS' ENTERED AT 12:38:17 ON 04 AUG 2008
                D STA QUE L74

     FILE 'WPIX' ENTERED AT 12:38:28 ON 04 AUG 2008
                D STAT QUE L75

     FILE 'ZCAPLUS, MEDLINE, EMBASE, BIOSIS, WPIX' ENTERED AT 12:38:45 ON 04
     AUG 2008
L79           43 DUP REM L78 L74 L75 (13 DUPLICATES REMOVED)
                      ANSWERS '1-43' FROM FILE ZCAPLUS
                D IBIB ABS HITIND L79 1-43

     FILE 'REGISTRY' ENTERED AT 12:39:58 ON 04 AUG 2008

     FILE 'ZCAPLUS' ENTERED AT 12:40:03 ON 04 AUG 2008
                D STAT QUE L9

     FILE 'CASREACT' ENTERED AT 12:40:13 ON 04 AUG 2008
                D STAT QUE L11

     FILE 'TOXCENTER' ENTERED AT 12:40:22 ON 04 AUG 2008
                D STAT QUE L13

     FILE 'PROUSDDR' ENTERED AT 12:40:30 ON 04 AUG 2008
                D STAT QUE L17

     FILE 'SYNTHLINE' ENTERED AT 12:40:40 ON 04 AUG 2008
                D STAT QUE L18

     FILE 'BEILSTEIN' ENTERED AT 12:40:50 ON 04 AUG 2008
                D STAT QUE L29

     FILE 'BABS' ENTERED AT 12:40:58 ON 04 AUG 2008
                D STAT QUE L24

     FILE 'ZCAPLUS, CASREACT, TOXCENTER, PROUSDDR, SYNTHLINE, BEILSTEIN, BABS'
     ENTERED AT 12:41:21 ON 04 AUG 2008
L80           22 DUP REM L9 L11 L13 L17 L18 L29 L24 (9 DUPLICATES REMOVED)
                       ANSWERS '1-15' FROM FILE ZCAPLUS
                       ANSWER '16' FROM FILE PROUSDDR
                       ANSWER '17' FROM FILE SYNTHLINE
                       ANSWERS '18-20' FROM FILE BEILSTEIN
                       ANSWERS '21-22' FROM FILE BABS
                D IBIB ABS HITSTR L80 1-15
                D IALL L80 16-17
                D IDE ALLREF L80 18-20
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D IALL L80 21-22

FILE HOME

FILE REGISTRY
Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 2 AUG 2008 HIGHEST RN 1037774-47-2
DICTIONARY FILE UPDATES: 2 AUG 2008 HIGHEST RN 1037774-47-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

FILE ZCAPLUS

FILE COVERS 1907 - 4 Aug 2008 VOL 149 ISS 6
FILE LAST UPDATED: 3 Aug 2008 (20080803/ED)

ZCAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE CASREACT

FILE CONTENT:1840 - 3 Aug 2008 VOL 149 ISS 6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

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*                                                          *
*     CASREACT now has more than 15.3 million reactions    *
*                                                          *
************************************************************
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In addition to reactions indexed by CAS, CASREACT contains reactions derived from the following: ZIC/VINITI database (1974-1999) provided by InfoChem; INPI data prior to 1986; Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich; organic reactions, portions copyright 1996-2006 John Wiley & Sons, Ltd., John Wiley and Sons, Inc., Organic Reactions Inc., and Organic Syntheses Inc. Reproduced under license. All Rights Reserved.

This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE TOXCENTER

FILE COVERS 1907 TO 29 Jul 2008 (20080729/ED)

The MEDLINE file segment has been updated with the National Library of Medicine's revised 2008 MeSH terms. See HELP RLOAD for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

The BIOSIS segment of TOXCENTER has been augmented with 13,000 records from 1946 through 1968.

FILE PROUSDDR

FILE COVERS 1980 TO 1 Jul 2008 (20080701/ED)

FILE SYNTHLINE

FILE COVERS 1984 TO 16 Jun 2008 (20080616/ED)

FILE BEILSTEIN
FILE LAST UPDATED ON April 1, 2008

FILE COVERS 1771 TO 2008.
FILE CONTAINS 10,322,808 SUBSTANCES

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For mo detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

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************************************************************
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST.      *
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* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE  *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE         *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.                       *
* FOR PRICE INFORMATION SEE HELP COST                               *
*********************************************************************

>>> Price change as of January 1st, 2008: Connect Time and Structure
    Search fees re-introduced. See NEWS and HELP COST <<<

FILE BABS
FILE LAST UPDATED: 14 JUL 2008       <20080714/UP>
FILE COVERS 1980 TO DATE.

FILE CHEMCATS

FILE LAST UPDATED 26 JULY 2008 (20080726/UP)

For details on recent updates in CHEMCATS, enter NEWS FILE at an arrow
prompt.  For the list of suppliers currently in the file, enter
HELP SPA, HELP SPB, HELP SPC, HELP SPDH, HELP SPIN, HELP SPOQ, HELP
SPRS, and HELP SPTZ.  For the list of current catalogs, enter
HELP CTA, HELP CTB, HELP CTC, HELP CTDH, HELP CTIL, HELP CTMN, HELP
CTOQ, HELP CTRS, and HELP CTTZ.

This database is provided on an "as is" basis.  Please consult the
suppliers for current information regarding pricing, regional
availability, available quantities, purities, etc.  THERE ARE NO
WARRANTIES OF ANY KIND, EITHER EXPRESSED OR IMPLIED.  ACS is not
liable for any loss of profit, goodwill or any other damages arising
out of the use of this database.

CHEMCATS now contains more than 23 million records.  See HELP CONTENT
and NEWS FILE for details.

FILE STNGUIDE
FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Aug  1, 2008 (20080801/UP).

FILE MEDLINE
 FILE LAST UPDATED: 3 Aug 2008 (20080803/UP).  FILE COVERS 1949 TO DATE.

  MEDLINE has been updated with the National Library of Medicine's
  revised 2008 MeSH terms.  See HELP RLOAD for details.

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.

  See HELP RANGE before carrying out any RANGE search.

FILE EMBASE
 FILE COVERS 1974 TO 4 Aug 2008 (20080804/ED)

 EMBASE was reloaded on March 30, 2008.

 EMBASE is now updated daily.  SDI frequency remains weekly (default)
 and biweekly.

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.
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Beginning January 2008, Elsevier will no longer provide EMTREE codes as part of the EMTREE thesaurus in EMBASE. Please update your current-awareness alerts (SDIs) if they contain EMTREE codes.

For further assistance, please contact your local helpdesk.

FILE BIOSIS
FILE COVERS 1926 TO DATE.
CAS REGISTRY NUMBERS AND CHEMICAL NAMES (CNs) PRESENT
FROM JANUARY 1926 TO DATE.

RECORDS LAST ADDED: 31 July 2008 (20080731/ED)

BIOSIS has been augmented with 1.8 million archival records from 1926 through 1968. These records have been re-indexed to match current BIOSIS indexing.

FILE WPIX
FILE LAST UPDATED: 31 JUL 2008 <20080731/UP>
MOST RECENT THOMSON SCIENTIFIC UPDATE: 200849 <200849/DW>
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE
>>> Now containing more than 1.1 million chemical structures in DCR <<<

>>> IPC Reform backfile reclassifications have been loaded to the end of March 2008. No update date (UP) has been created for the reclassified documents, but they can be identified by 20060101/UPIC and 20061231/UPIC, 20070601/UPIC, 20071001/UPIC, 20071130/UPIC and 20080401/UPIC.
ECLA reclassifications to April and US national classifications to the end of January 2008 have also been loaded. Update dates 20080401/UPEC and /UPNC have been assigned to these. <<<

FOR A COPY OF THE DERWENT WORLD PATENTS INDEX STN USER GUIDE,
PLEASE VISIT:
http://www.stn-international.de/training_center/patents/stn_guide.pdf

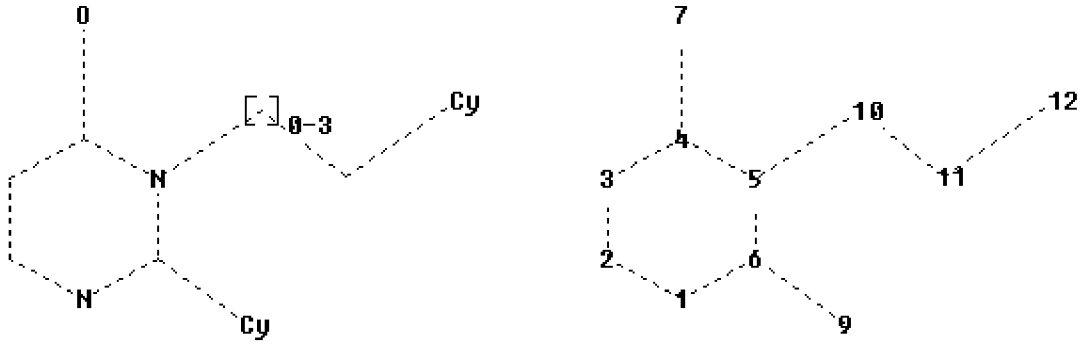
FOR DETAILS OF THE PATENTS COVERED IN CURRENT UPDATES, SEE
http://scientific.thomsonreuters.com/support/patents/coverage/latestupdate

EXPLORE DERWENT WORLD PATENTS INDEX IN STN ANAVIST, VERSION 2.0:
http://www.stn-international.com/archive/presentations/DWPIAnaVist2_0710.p

>>> HELP for European Patent Classifications see HELP ECLA, HELP ICO <<<

>>> Please note that the COPYRIGHT notification has changed <<<

Uploading L1.str

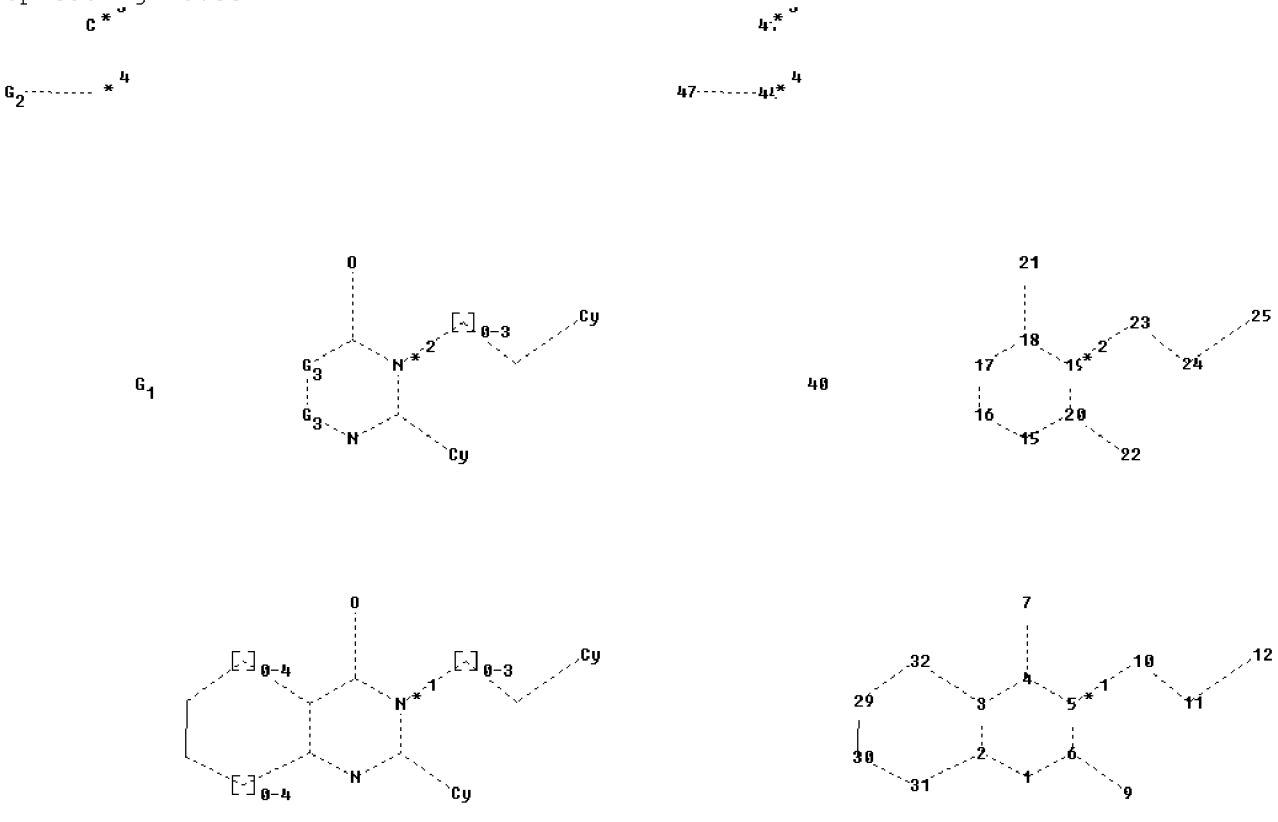


chain nodes :
7 9 10 11 12
ring nodes :
1 2 3 4 5 6
chain bonds :
4-7 5-10 6-9 10-11 11-12
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
1-2 1-6 2-3 3-4 4-5 4-7 5-6 5-10 6-9 10-11 11-12

Connectivity :
4:3 E exact RC ring/chain 6:3 E exact RC ring/chain 7:1 E exact RC ring/chain

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 9:Atom 10:CLASS 11:CLASS 12:Atom
Generic attributes :
9:
Saturation : Unsaturated
12:
Saturation : Unsaturated

Uploading L6.str



chain nodes :
7 9 10 11 12 21 22 23 24 25 40 47

```
ring nodes :
1  2  3  4  5  6  15  16  17  18  19  20  29  30  31  32  41  44
chain bonds :
4-7  5-10  6-9  10-11  11-12  18-21  19-23  20-22  23-24  24-25  44-47
ring bonds :
1-2  1-6  2-3  2-31  3-4  3-32  4-5  5-6  15-16  15-20  16-17  17-18  18-19  19-20
29-30  29-32  30-31
exact/norm bonds :
1-2  1-6  2-3  2-31  3-4  3-32  4-5  4-7  5-6  5-10  6-9  10-11  11-12  15-16  15-
20
16-17  17-18  18-19  18-21  19-20  19-23  20-22  23-24  24-25  29-32  30-31  44-47
exact bonds :
29-30
isolated ring systems :
containing 15 :


G1:[*1],[*2]

G2:X,Cy,Ak

G3:[*3],[*4]

Connectivity :
4:3 E exact RC ring/chain  6:3 E exact RC ring/chain  7:1 E exact RC ring/chain
18:3 E exact RC ring/chain  20:3 E exact RC ring/chain  21:1 E exact RC ring/chain
41:2 E exact RC
ring/chain
Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:CLASS  9:Atom  10:CLASS  11:CLASS
12:Atom  15:Atom  16:Atom  17:Atom  18:Atom  19:Atom  20:Atom  21:CLASS  22:Atom
23:CLASS  24:CLASS
25:Atom  29:Atom  30:Atom  31:Atom  32:Atom  40:CLASS  41:Atom  44:Atom  47:CLASS
Generic attributes :
9:
Saturation             : Unsaturated
12:
Saturation             : Unsaturated
22:
Saturation             : Unsaturated
25:
Saturation             : Unsaturated




=>
```